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Terascale Simulation Tools and Technologies

TSTT

The Terascale Simulation Tools and Technologies Center Annual Report

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1 Overview

The overall goal of the TSTT Center is to enable the scientific community to more easily use modern high-order, adaptive, parallel mesh and discretization tools. To achieve this goal, we are following three distinct but related paths. The first is to work directly with a number of lead application teams (for the most part SciDAC-funded) to use such technologies in their application domains. The second is to create new technology that eases the use of such tools, not only for our designated application partners, but across a broad range of application areas that require mesh and discretization tools for scientific simulation. The main technology thrust is not to create new tools (although some of this will occur), but to create new capabilities that will allow the use of these tools interoperably. This very profound step can be compared to the shift from hand craftmanship to manufactured products with interchangable components which revolutionized the world economy one to two centuries ago. The third component of our efforts is to embed this work in a larger framework of related activities, each seeking a similar, and profound, change in the practice of computational science.

To ensure the relevance of our work to the SciDAC program goals, we originally selected six application areas, and in each, one or more application projects and teams with which to work directly. One application collaboration which targeted the development of an adaptive mesh refinement capability for the oceanographic code POP was postponed and may be dropped due to unanticipated technical obstacles in the specific goal selected. One new application involving jet breakup for spray combustion was added. The initial job of establishing good working relations, agreement on a plan of action, and obtaining initial results was accomplished in all cases. In general, our work with the applications has been more difficult than anticipated, in spite of the experience of the TSTT team members in similiar application-motivated collaborations. For this reason, the routes to the goals have been modified in some cases, but good progress has been obtained for all of the targeted application teams. For example, in the case of the electromagnetic code for accelerator design, the original goal of developing more stable meshes has been enlarged to include the underlying difficulty which motivated this goal: to cure or ameliorate instabilities of the time stepping algorithm. With the fusion M3D code, we decided to work initially with a related, but smaller and more easily modified code from the same application team, for initial testing and proof of principle, as the full M3D code proved difficult to work with. In several applications (astrophysics, climate), our initial technology development goals were met, and while we await their use or evaluation, further collaborative goals will be pursued. The spray breakup problem achieved initial success and awaits adaptive TSTT technology to allow refined grid simulations for its next steps. We plan to continue the intensive effort to insert our existing advanced mesh and discretization technology into existing application codes for the coming year.

Our main progress towards the development of new technology has been the definition of the low level interface to a variety of mesh generation and adaptive mesh management tools. This interface provides a common calling convention that will allow an application to call any compliant mesh tool in an interchangeable fashion. Most of the TSTT advanced meshing tools have been or will be made compliant to this interface. We have also pursued one-on-one interoperability goals with the development of interoperability between the FronTier front-tracking library and the Overture mesh library. This goal, advanced from year two to year one because of its need in one of our applications, has made good progress, and will be completed in the coming year.

Finally, we mention the integration of this effort (interoperability and applications) with a larger computational science effort. The importance of this broader integration goal can be understood by recalling our larger goal of influencing the practice of computational science in a general sense. We have engaged the computational science community with an invitation to comment on our interoperability plan. In particular, we have interacted several times with two related projects that are defining common interfaces. The first is the NSF-funded Mississippi State/Cornell project on adaptive algorithms which is working to define a new standard for geometric descriptions and the second is the Unstructured Grid Consortium which is working to define interfaces and data structures that allow interchangeability in mesh generation algorithms. We have also been assiduous in meeting and planning with our applied mathematics and computer science partner ISICS. The APDEC ISIC, which emphasizes interfaces for patched-based AMR schemes, is targeting a sub-goal of the TSTT interface definition effort. Thus we will ensure that their interface standards are consistent with and can be subsumed within our own. The other centers are following our work and we are following theirs. We hope to ensure smooth working relations, and to the extent practical, compatibility of tools. We have presented our work to the computational science community and will continue to do so. We hope in this manner to achieve a broad acceptance for our goals and for the route we are following to achieve them.

2 FY02 Accomplishments

We have made considerable progress in the past year, both with respect to our goal to demonstrate the use of TSTT technology in SciDAC application problems and with respect to our long-term technology goal of creating interoperable and interchangeable meshing and discretization components. The table below contains a summary of our progress with respect to our deliverables as stated in the TSTT proposal.

In general, our work with the applications teams is more extensive than originally planned. In the proposed milestones, we had targeted three application areas in year one; in reality we are working with a mucher broader spectrum. The additional effort in this area is attributed to the recognition that these collaborations are critical for the success of the SciDAC program. In the technology area, several of our efforts are on track. In particular the development of the Mesquite mesh quality improvement toolkit and the low level common interface are progressing well. Two of our technology goals have been delayed. First, the design and development of the discretization library depends on the completion of the low-level mesh interface. Thus we have postponed the development of the initial design for this library, but work at individual sites to lay the necessary groundwork is underway. In addition, we have postponed the development of FrontierLite in favor of the Frontier-Overture merge to create new capabilities needed by one of our application partners. Finally, we have eliminated two of our deliverables, namely those pertaining to structured mesh generation and dynamic load balancing, due to budget revisions.

FY02 Proposed	FY02 Accomplished	Comments
Initial definition and deployment of low level interfaces for mesh and field data	Initial definition of low level mesh interface	Field interface definition to be done with discretization operators; Mesh interface implementation not complete
Design and initial implementation of discretization operator library	Design of DO library postponed to late FY02. Underlying code for DO's implemented for structured (LLNL) and unstructured (RPI) meshes	DO library design postponed until mesh interface definition complete
Development of a priori mesh quality assessment and improvement tools for unstructured and structured meshes	Mesquite development is on track; developed a flexible code design that is implemented in version .5	
Structured mesh generation improvement to increase speed and functionality	N/A	Deliverable eliminated due to budget cut
Extraction of the essential algorithms and routines from FronTier to begin implementation of a stand-alone front tracking software package, FronTier-Lite	Delayed in favor of Frontier-Overture merger	FronTier-Lite will be developed after AMR capabilities are incorporated in FronTier
Insert existing discretization and mesh generation methods into fusion, accelerator and chemistry applications	RPI assessing potential for higher order FEM methods for fusion effort at PPPL LLNL researching stabilized versions of DSI scheme for tau3P code at SLAC, SNL generating meshes for tau3p BNL developing front tracking code for jet breakup.	Other application work includes collaborations with the climate and biology communities.
Begin to examine how to employ information on the mesh hierarchy for the effective construction of the parallel decomposition (level 3)	Some initial work in this area is progressing as part of the RPI effort. No focused efforts have occurred yet.	
Extend existin g dynamics load balancing technologies to effectively account for heterogeneous parallel computing environments	N/A	Deliverable eliminated due to budget cut
Make a preliminary assessment on how hierarchical information we generate may be exploited in downstream applications, focusing on iterative solver technology under development in related ISIC's	Preliminary discussions have been had with the TOPS center, but no focused efforts are underway at this time	
Hire software engineer, set up web site repository, cvs, autoconf, and establish a coding standard	All but the coding standard	A coding standard unlikely to happen, we are more interested in the development of a common interface rather than imposing a standard on TSTT tools

2.1 Applications

In this section, we highlight the results of our most promising interactions with the SciDAC application teams. We have invested a significant portion of our resources in meeting with scientists from each of the SciDAC application areas, analyzing their needs for advanced meshing and discretization technologies, and working with them to demonstrate the promise of such techniques in their application domains. We highlight these interactions here; more details can be found in Sections 2.1.1-2.1.6.

- For accelerator design, we have focused on helping to increase the stability of the Tau3P simulation code used for computational electromagnetics simulations at SLAC. We have adopted a two-pronged approach. First, we are seeking to understand the dependence of the simulation code stability on properties of the meshes used for accelerator design simulations and are using TSTT mesh generation technology to shorten the time required to generate high-quality, all-hexahedral meshes. Second, we are working to understand and improve the stability of the simulation code by analyzing the DSI discretization strategy used in Tau3P. Early successes of this work include the construction of a stable, first-order accurate method for triangular meshes and the ability to stabilize the DSI scheme by adding high-order artificial dissipation. Because the addition of artificial diffusion can affect long term accuracy of these simulations, more work is needed to complete this aspect of the project.

- For two of the astrophysics SciDAC centers, we have demonstrated the potential impact of high-order discretization methods for both the hydrodynamics and neutrino transport aspects of their simulations. In both cases, adaptive Discontinuous Galerkin discretizations were implemented for the appropriate test problems and comparison to the currently used techniques shows that a significant benefit in terms of accuracy and time to solution can be obtained by using these techniques.

- In our interactions with climate scientists, we have focused our efforts in two main areas. First, we have worked on mesh generation strategies which create high-quality grids whose vertices are focused over regions of interest, and, in this case in particular, over regions of high altitude. Second, joint work between scientists at NCAR and at ANL has resulted in a new preconditioner for spectral element simulations based on low-order finite element discretizations that has accelerated the integration rate in the shallow water equations test problem.

- TSTT members at BNL and SUNY SB have been working with scientists at Argonne to create a simulation code that models spray formation in diesel jet break up using an enhanced version of the FronTier front-tracking code. Early simulation results have helped determine the sensitivity of the model to various input parameters and is a primary motivator for our work to create interoperable meshing technologies.

- In our work with fusion scientists at PPPL, we have targeted the use of high-order adaptive discretization technologies in MHD fusion simulations. To date, we have examined the M3D code to determine if it can be installed at SCOREC, implemented a specific MHD capability within the SCOREC Trellis framework, and tested this capability with an appropriate test problem. This work provides the foundation for the algorithms that we plan to directly insert into the M3D code.

- We are also working to cultivate a relationship between TSTT and computational biologists by incorporating TSTT technology into two DOE programs in this area. The focus of our efforts are in image reconstruction and feature extraction for complex biological systems, and we have had initial successes in microbial cell and human lung modeling along with geometry extraction and mesh generation for rat olfactory systems.

2.1.1 Accelerator Design

TSTT Personnel: David Brown (LLNL), Kyle Chand (LLNL), Bill Henshaw (LLNL), Patrick Knupp (SNL)

Accelerator Personnel: Nate Folwell (SLAC), Kwok Ko (SLAC)

TSTT interactions with the SciDAC *Advanced Computing for 21st Century Accelerator Science and Technology Center* have been primarily focused on the computational electromagnetics group headed by Kwok Ko at the Stanford Linear Accelerator (SLAC).

The primary codes used for electromagnetic simulations are a frequency domain code (Omega3P) and a time domain code (Tau3P). At the August 2001 SciDAC Accelerator Kickoff meeting, Ko presented a number of outstanding problems related to meshing and discretization for which he hoped the TSTT Center would be able to provide assistance. The first problem is the widely recognized issue of reducing the time needed to create a mesh starting with a CAD (computer-aided design) model giving the physical geometry for the simulation. There are two main bottlenecks involved in this process—one is the clean-up of the initial geometry such that it can be used for mesh generation. The second bottleneck (for SLAC) concerns the generation of high quality meshes as it relates to accuracy and convergence of the simulation code. Currently, many meshes may be generated before a successful simulation is obtained.

The geometry clean up process consists of removing unwanted detail, healing gaps between surfaces and volumes, and removing non-physical overlaps. This process can be quite tedious and time-consuming, often delaying simulations for months. Both CUBIT (SNLA) and Overture (LLNL) have tools available for CAD cleanup and repair. SLAC has been using the CUBIT tools for some time, and TSTT will provide the Overture "Rapsodi" cleanup tools to SLAC in the near future. In addition, TSTT members have been assisting SLAC in the use of these tools. For example, toward the end of FY02, SLAC presented a very complex tapered waveguide geometry that needed to be cleaned up and meshed as quickly as possible (see Figure 1). The challenge in this geometry is that the position of the beam axis relative to the centroid of the geometric cross-section varies along the waveguide which makes it difficult to achieve sufficient mesh quality. Tim Tautges at SNL/TSTT has been working with the SLAC analysts to clean up this geometry and mesh it using CUBIT. Although this work is not completed, it appears that there will be a major reduction in the time it would have taken the SLAC analysts to mesh this problem themselves.

The second problem posed by Ko concerned Tau3P. The code uses the DSI (Discrete Surface Integral) method which is known to be weakly unstable on non-orthogonal meshes. Because of the complexity of the geometries required for accelerator design, it is not possible, in general, to generate meshes that are completely orthogonal. Although Tau3P partially stabilizes the DSI method by invoking a time-domain filtering technique, the overall simulation process is not very robust because simulations must often be terminated prematurely at some "cutoff" time due to instability. A much more desirable situation would be to have a stable method where the only quality issue would be the accuracy of each simulation.

SLAC analysts have long observed that the cutoff time is highly sensitive to mesh properties such as orthogonality and smoothness. Based on the hypothesis that the Tau3P cutoff time might be correlated to some measure of quality of the mesh used in the calculation, a collaboration was started between N. Folwell (SLAC) and P. Knupp (SNLA), to systematically identify the major correlations between cutoff time and mesh properties. An empirical study showed that there were strong correlations between cutoff time and mesh properties such as smoothness, element shape, and the minimum edge length. The strength of the correlations varied depending on whether a calculation used the Tau3P filtering technique or not; it also depended on whether the simulation involved a beam or a pulse. This work is nearing completion. Results will be used in FY03 to aid the creation of better (more stable) meshes for SLAC.

More recently, we have also begun a study of the DSI (and similar) methods with the goal of stabilizing the underlying discretization. At LLNL, Bill Henshaw has been studying DSI-like methods as applied to wave equations in general to see if this might be possible. Preliminary results have included the derivation of sufficient conditions for stability of the method on triangular meshes in 2D. We understand how to construct a first-order accurate method that is stable on triangular meshes, and also how to stabilize DSI by adding high-order artificial dissipation. Further work will be required to develop techniques that will perform well on general meshes for 3D electromagnetic simulations.

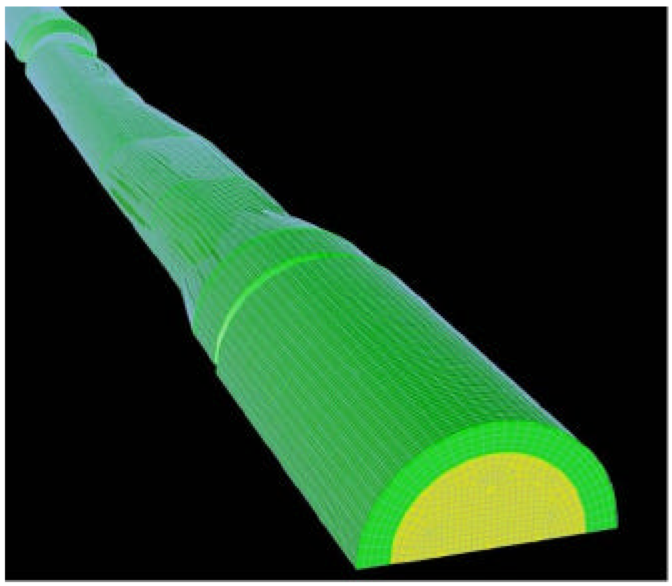


Figure 1 An all-hexahedral mesh generated for the SLAC waveguide geometry

2.1.2 Astrophysics

TSTT researchers at ORNL and RPI have active collaborations with two astrophysics SciDAC centers: the Terascale Supernova Initiative (TSI) led by Mezzacappa and the Magnetic Reconnection Center led by Bhattacharjee. The primary focus in both cases is the exploration of alternative discretization strategies for various aspects of the solution process including the neutrino transport problem and hydrodynamics simulations. In addition, we have been exploring a 3D spatial caching strategy to reduce costly evaluations of the scattering kernels for Boltzman transport.

Discontinuous Galerkin Discretizations for Radiative Transfer

TSTT Personnel: Valmor de Almeida (ORNL), Ed D'Azevedo (ORNL)

Astrophysics Personnel: Tony Mezzacappa (ONRL), Bronson Messer (ORNL), Matthias Liebendoerfer (ORNL)

With the TSI team, TSTT researchers at ORNL are exploring new schemes for solving models of radiative transfer in stellar atmospheres representative of supernova type 2 core collapse/explosions. The current solution method, namely, discrete ordinates, in conjunction with finite differences, may require petascale computing power when extended to three dimensions. The TSTT/TSI interaction is aimed at exploring novel schemes that are able to keep computational requirements at the terascale level.

A series of radiative transfer prototype problems have been chosen by the TSI group. These problems are simplified forms of Boltzmann's integro-differential equation for radiative transfer and thus have features significant to supernova collapse/explosion modeling.

The first problem, Milne's axis-symmetric pure scattering of photons in extended stellar atmospheres, has been studied successfully. In this problem the dependent variable is the radiative intensity field (photon distribution function), and the independent variables are the radius of the spherical stellar atmosphere and the polar angle made by the radius and the photon velocity vector. The new method of analysis consists of a discontinuous Galerkin (DG) approach for the approximation of the radiative intensity field in phase space (the Cartesian product of the one-dimensional radius domain and the polar angle domain). The integro-differential equation is treated as a linear hyperbolic PDE at each step of an iterative scheme that corrects the value of the integral scattering kernel. Each iteration is accelerated by evaluating the kernel from the first and zeroth moments of the original problem. The DG method applied to the linear hyperbolic problem at each iteration was implemented explicitly in phase space since the characteristic curves are known a priori. This allows the resulting linear algebraic set of equations to be solved locally and progressively along wave fronts normal to the characteristics. The DG method developed for the Milne's problem was found to be memory efficient (requiring one order of magnitude less storage than the discrete ordinate method) and fast (one order of magnitude faster than DOM). In addition, in view of the adaptive mesh used, the results were significantly more accurate when capturing important features of the solution. For instance, the region of transition from diffusive radiation to streaming was correctly captured, and the outward peaking (a delta function like sharp increase) of the radiation field at the outer boundary of the extended atmosphere was correctly reproduced. The results were obtained for a range of atmosphere sizes including the range of interest to supernova applications. Although the results are exciting, supernova models are significantly more complex, involving the extended set of equations that couple neutrino radiation transfer to relativistic flow, that is radiative hydrodynamics.

Discontinuous Galerkin Discretizations for Hydrodynamics

TSTT Personnel: Mark Shephard (RPI), Joe Flaherty (RPI), Jean-Francios Remacle (RPI)

Magnetic Reconnection Personnel: Robert Rosner (UofC), Greg Weirs (UofC), Andrew Seigel (UofC)

The TSTT team at SCOREC (RPI) is working with the astrophysicists at the University of Chicago to develop *hp*-adaptive discontinuous Galerkin discretizations for flow problems of importance to astrophysics applications. This work is part of a long-standing collaboration with the FLASH center at the UofC and is currently funded by both the ASCI ASAP program and

SciDAC. The work outlined in this section was funded predominantly by the ASCI ASAP program, but lays the groundwork for new research that will be funded by SciDAC.

Together with the FLASH team, we determined a set of test problems that would provide a basis of comparison between h-p adaptive DG methods and the currently used Piecewise Parabolic method. With the start of the SciDAC program, we executed these test problems in the SCORE Trellis framework—a flexible, extensible framework for PDE-based application solution. We ran the tests on both uniform meshes and adaptive meshes to demonstrate the increased efficiency over fixed grids.

Based on these and other studies, the *h*-adaptive techniques in the DG code have been extended in terms of capability and efficiency. Both nonconforming isotropic and conforming refinement strategies are now supported and the conforming refinement includes an initial anisotropic mesh adaptation using an anisotropic error indicator. These tests also showed that the effective application of *p*-adaptivity requires additional developments in two areas. The first is the appropriate adaptive selection of polynomial order. The second and more difficult task is the construction of a reliable high-order limiting method which works in the general 3D case. This is particularly crucial for hyperbolic equations such as the Euler equations because of shocks and discontinuities. Limiting the solution at the vicinity of discontinuities is always required but usual limiting techniques have the major drawback of reducing the accuracy of the solution in regions where a limiter is not be required. We developed an error estimator for DG based on superconvergence of the solution (in average) at outflow boundaries. Using that important result, we developed a robust shock detector that enables us to turn on/off the limiter procedure when needed. Figure 2 shows an example of the computation of vortex sheets using the detector.

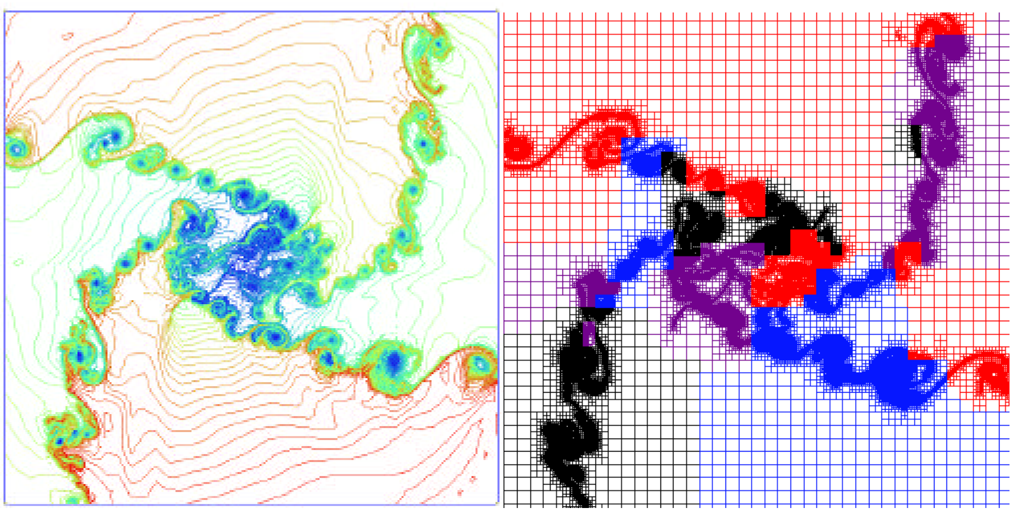


Figure 2 Density contours (left) and adapted mesh (right) for the vortex sheet problem at t=1.

Efforts are now being initiated to integrate DG discretizations, local time stepping and a TSTT mesh interface into the FLASH code. In previous work, a distributed memory, explicit local time stepping technique was developed as the integration scheme used with the DG discretization. This scheme allows us to satisfy the Courant (CFL) stability condition locally rather than globally and efficiencies are often 50 to 100 times those of methods using a single time step in a method of lines formulation. This scheme provides accurate resolution near shocks and other discontinuities. It is also useful for resolving layers in viscous problems with small diffusion.

The DG methods extend to viscous problems while conserving the higher order of accuracy, and we think this method is worthwhile for such a class of problems. We are planning to consider an implicit in time integration scheme to enhance the capabilities of the code to solve problems of interest to the FLASH project, such as wave breaking problems or double diffusion. Our experience in using TOPS solvers such as PETSc will help us to provide such capabilities. For DG, a matrix free GMRES type method might be suitable and also very efficient. The compactness of the DG stencil might permit some very simple block diagonal preconditionings (e.g., local Jacobi methods). Using the DG method for implicit time integration is another very interesting possibility that we will explore.

Caching Strategies for Boltzman Transport

TSTT Personnel: Ed D'Azevedo (ORNL)

TSI Personnel: Bronson Messer (ORNL)

Another interaction between TSTT and TSI is the use of a 3D spatial cache for avoiding redundant and costly evaluations of scattering kernels for Boltzmann transport. The scattering kernel is a function of density, temperature and species fraction. We have generated trace data over a realistic TSI computation and visualized the trajectories of evaluation in 3D phase space (density, temperature, species fraction). Initial analysis shows 3D interpolation with a small global cache has good hit ratio of over 90%, or about 9 of 10 evaluations of scattering kernels can be computed by 3D interpolation instead of the actual costly computations.

2.1.3 Climate

In our interactions with climate scientists, we have focused our efforts in two main areas. First TSTT scientists at ORNL have been working on strategies to create high-quality meshes whose grid points are focused over regions of interest, in this case, over regions of high altitude in the world. Second, joint work between scientists at NCAR and at ANL has resulted in a new preconditioner for spectral element simulations based on low-order finite element discretizations.

Smooth Grid Refocusing

TSTT Personnel: Ahmed Khamayseh (ORNL)

Climate Personnel: John Drake (ORNL), Daniel Guo (North Carolina at Wilmington, formerly of ORNL)

The accuracy and convergence of computational solutions using mesh-based numerical methods are strongly dependent on the quality of the mesh being used. Our efforts at ORNL and part of TSTT efforts include the development of several algebraic and PDE-based elliptic methods for optimizing meshes that are comprised of elements of arbitrary hybrid polygonal and polyhedral type. These methods provide the ability to generate and focus mesh resolution over areas of particular interest yet strive to equidistribute the node densities of the mesh while improving the aspect ratios and quality of mesh cells. The numerical methods that solve the partial differential equations perform node redistribution on the mesh to maximize the equidistribution of a weighted function of geometric and solution parameters.

Applications of this capability include the generation and adaptation of smooth grid transformations for General Circulation Models (GCMs) that attempt to simulate the Earth's climate system. Mesh adaptation can play a crucial role in atmospheric-ocean-land models that calculate physical quantities such as temperature, humidity, wind speeds which have direct effect on sea ice cover, soil moisture, and cloud formation. In climate modeling, mesh adaptation can also reduce the simulation error in prediction of (1) the dynamics of the climate system that describe the large-scale movement of air masses and transport of energy and momentum; (2) the physics of the climate system such as radiation transmission through the atmosphere, thermodynamics, and evaporation; and (3) other factors such as air-sea interaction, topography, and vegetation parameters.

Our efforts in this area have focused on developing two adaptive methods for climate modeling and simulation. The first method developed is an algebraic method in which the mesh is adapted to reduce the error in the solution while the mesh remains orthogonal. This method works on logically structured meshes where the mesh is first adapted along the boundaries of the domain and then algebraically interpolated into the interior. The second method is based on solving an adaptive elliptic mesh generation system coupled with the climate physical model. These methods are currently utilized at ORNL for the generation of refocused adaptive meshes applied to fine scale processes in climate modeling. In particular, we concentrated our efforts on producing high quality meshes that are adapted to the earth's orography field, i.e., earth's surface height. We have generated a variety of meshes (structured and unstructured) with the feature of mesh refocusing in and around areas high altitude without changing the resolution of the initial meshes (see Figure 3). In return, the pay off in computational cost is reduced while achieving the desired simulation results. The climate code would spend much less computational time using adapted optimized mesh to obtain a high quality solution verses using non-adapted mesh.

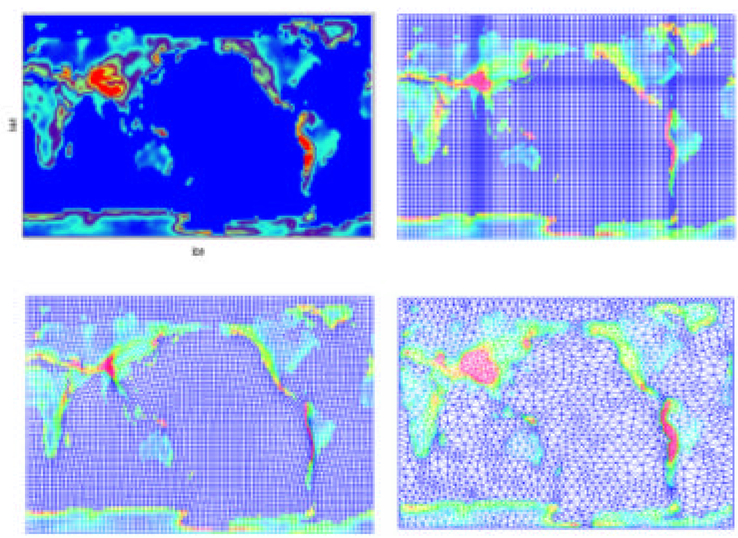


Figure 3 Meshes adapted to the earth's orography field

Low-Order Discretizations used as Preconditioners

TSTT Personnel: Paul Fischer, Henry Tufo (ANL)

Climate Personnel: Steve Thomas, J. Dennis (NCAR)

Climate and weather models have traditionally been based on spectral methods that exploit the underlying symmetries of spherical geometry by representing the solution as a tensor product of global basis functions. Such methods provide a high degree of accuracy per grid point and, through the use of transforms, make the implicit steps of the underlying PDEs easy to solve. Unfortunately, the transforms, needed for both operator evaluation and inversion, require all-to-all communication on multicomputers, which is a potential bottleneck on systems having limited bisectional bandwidth. Spectral element methods (SEMs), which employ *local* spectral expansions interior to quadrilateral or hexahedral elements, offer another approach to achieving the high degree of numerical accuracy required for long time integrations typical of climate simulations. The SEM discretization requires only C^0 continuity and hence has low communication requirements. The spectral element method has been proven effective in geophysical fluid dynamics (GFD) by Iskandarani et al. (1995), Taylor et al. (1997), and by Thomas and Loft (2002).

The ANL TSTT group has been working with Thomas and Loft at NCAR to further develop semi-implicit spectral element methods for GFD. We have been investigating finite-element-(FE-) and block-Jacobi-based preconditioning strategies for a semi-implicit treatment of the shallow-water equations that is designed to overcome the timestep-size restrictions imposed by fast gravity waves. The FE-based preconditioner exploits the spectral equivalence between the high-order SEM discretization and a low-order FEM discretization based on the same set of interpolation points. We have shown (Thomas et al., 2002) that, at moderately high resolution, the FEM-based approach, coupled with an additive overlapping Schwarz strategy, outperforms block-Jacobi preconditioning, even in large-scale parallel environments. We are currently investigating the potential of a two-level additive Schwarz method, in which the preconditioner is augmented with a coarse-grid problem. The coarse-grid problem is defined by discretizing the original PDE using bilinear interpolants on each spectral element.

2.1.4 Basic Energy Sciences (Combustion)

TSTT Personnel: James Glimm (BNL/SUNY SB), Wonho Oh (BNL), Roman Samulyak (BNL), Myoung-Nyoun Kim (BNL), Andréa Marchese (BNL), Xiaolin Li (SUNY SB)

Combustion Personnel: Constantine Tzanos (ANL)

TSTT members at BNL and SUNY SB have been working with scientists at Argonne to create a simulation code that models spray formation in diesel jet break up. This is an important aspect of the problem as it provides input to spray combustion models and is critical for predictive modeling of diesel engine combustion. The overall goal of such an effort is the design of a nonpolluting, fuel-efficient engine.

Spray formation is a difficult problem for simulation due to

- the geometric complexity and multiscale nature of the spray,

- the stiff equation of state (EOS) for diesel fuel, and the need to model phase transitions, shock waves and other strong hydrodynamic transients,

- the limited resolution of experimental diagnostics, and

- the sensitive dependence of spray formation on nozzle geometry and other problem parameters.

To model this process, we are using the front tracking code, FronTier which has a high quality interface capability that enables multiscale resolution of complex geometries. For this simulation, we enhanced FronTier with an Equation of State (EOS) module that supports diesel fuel with cavity formation (phase transitions). Using the enhanced version of the code and the flow geometry shown in Figure 4, we performed an initial exploration of input parameters that have a sensitive influence on the jet and its breakup. We found the following to be important:

- The diesel EOS. See Figure 5.

- The boundary conditions inside the nozzle. The flow in the nozzle appears to be turbulent, and the boundary conditions (varying between slip and no slip) should be set according to grid resolution.

- The rise time of the initial pressure transient (valve opening time).

- The diesel viscosity.

- The diesel meniscus at the nozzle outlet.

- The inlet pressure.

Our simulations are compared to measurements performed on the light source at ANL. In contrast to conventional (optical or photographic data), the light source can penetrate the spray and give data on local densities within the spray. It has thus settled the question (negatively) of an intact liquid core to the jet. The light source data thus gives volume fraction data through out the jet, as a function of time, distance down stream from the jet nozzle and distance from the central axis of the jet. Data from conventional instruments is also available, such as the positions (and velocities) of the tip and tail of the jet. The primary diagnostics are jet tip and tail velocities, and the volume fraction or mass density at various time and space localized cross sections of the jet.

Our present success is semi quantitative. See Figure 6. Due to the importance of the turbulent flow in the very narrow nozzle, further progress will require automatic mesh refinement (AMR), currently being added to FronTier through a merge with the Overture code (see section 2.2.1.3).

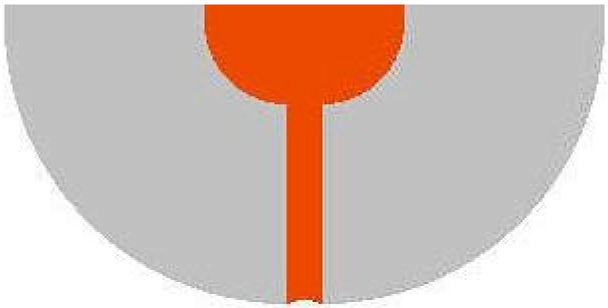


Figure 4 Layout of diesel jet. The upper flow region is a reservoir of diesel fuel, joined by a narrow nozzle to the engine combustion chamber below.

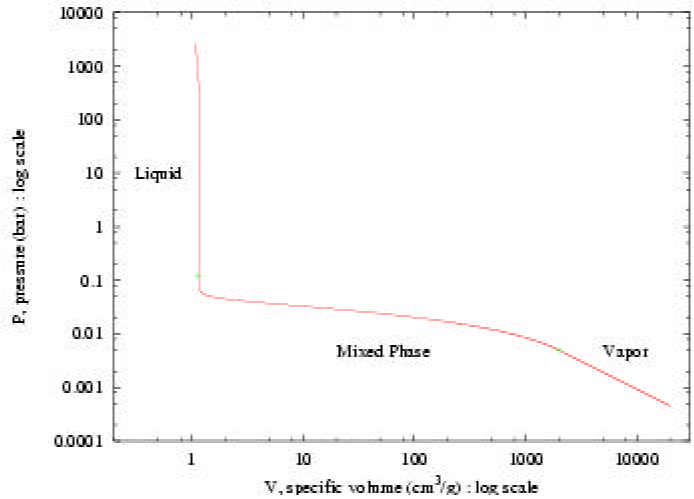


Figure 5 Plot of the pressure vs. specific volume isentrope for the diesel EOS. The approximate breaks in the slope of the curve mark the locations of the two edges separating the mixed phase region from the two pure phase regions (left, gas; right, liquid).

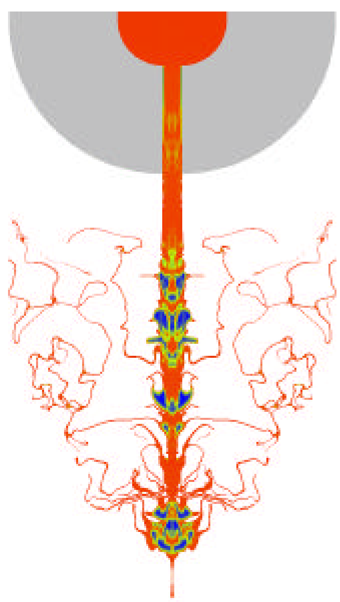


Figure 6 Partial breakup of the diesel jet after injection for a distance of 3.9 mm into the combustion chamber. Blue denotes diesel vapor, red is liquid, and green/yellow is a mixed phase region.

2.1.5 Fusion

TSTT Personnel: Katia Pinchedez (RPI), Shrinivas Lankalapalli (RPI), Jean-Francois Remacle (RPI), Joseph Flaherty (RPI) and Mark Shephard (RPI)

Fusion Personnel: Steve Jardin (PPPL), Hank Strauss (PPPL), Jin Chen (PPPL)

The goal of this effort is to develop high-order adaptive discretization technologies aimed toward solving MHD problems of importance to the fusion community. Efforts to date have involved examining the M3D code used at PPPL with an eye toward its installation at SCOREC and implementing a specific MHD capability within the SCOREC (RPI) Trellis framework to provide an initial demonstration of the type of procedures that can be developed.

The first activity included examining the M3D code for the purposes of (i) gaining a better understanding of the class of MHD problem being solved by PPPL, (ii) gaining an initial understanding of the numerical methods used in M3D and the methods of implementation used, (iii) determining the level of effort required to install M3D on the SCOREC computer system. An important lesson learned during this process is that the class of problems solved by M3D requires the application of advanced methods and that because of the evolutionary implementation of these methods, there is a complex interaction of the numerical methods, discretization technologies, and (parallel) computing environment. To effectively implement high-order and adaptive methods into M3D requires a stronger separation of the discretization library operations and the specific numerical methods used to solve the discretization. Due to the complexity of the class of problem being solved, it is not known in advance how easily or effectively those tasks can be undertaken.

As the first concrete step toward our long term goal, the SCOREC team has implemented one specific set of MHD equations previously considered by Hank Strauss and D. Longcope (J. Comp. Physics, 1998, 147) in the Trellis simulation system. Trellis is a geometry-based system for the implementation of high-order adaptive methods which already includes various high-order basis functions and allows the effective implementation of new weak forms and their discretization. The code is modular and individual components developed as part of this effort be transferred to and re-used in other simulation codes.

Using Trellis, we have investigated the two-dimensional, incompressible MHD equations in both the primitive variable formulation and stream function formulation. In our incompressible MHD model, both magnetic and velocity fields are solenoidal (divergence free) and there are two ways to enforce this constraint; (i) from the interior, using potentials, and (ii) from the exterior, using Lagrange multipliers.

We first used Lagrange multipliers to impose the incompressibility constraints because the magnetic part of the MHD model was trivial to add to our existing incompressible Navier-Stokes implementation in Trellis. We used semi-implicit time discretization and compute convective terms explicitly so that the stability in time is constrained by a CFL condition based on the fluid velocity. We used 2^{nd} and 3^{rd} order finite elements to discretize the primary fields (velocity and magnetic field) and spaces that are compatible with the Babuska-Brezzi conditions for the Lagrange multipliers. We were able to produce stable results on different grids and this first experiment enabled us to familiarize ourselves with MHD flows phenomenology.

In the stream function formulation, the equations consist of two Poisson equations and two time dependent nonlinear equations, one purely advective and the other advective diffusive. The nonlinearity is present in the form of Poisson brackets between two variables. In the weak form, the two time dependent equations are stabilized using the Streamline Upwind Petrov Galerkin (SUPG) method. Finite elements based on the Lagrange shape functions are used to discretize the weak form in space and a Backward Euler scheme is used for the time integration. The solution procedure consists of solving one equation at a time. This allows us to linearize the nonlinear terms in the equations by using values at the previous time steps for one of the variables in the Poisson bracket.

Our test case is the tilt instability example (Figure 7) studied by Strauss and Longcope for the incompressible case and by Richard, Sydora and Ashour-Abdalla for the compressible case. The initial equilibrium state corresponds to a bipolar vortex for the magnetic field with zero initial velocity for the fluid. Two oppositely directed currents are embedded in a constant magnetic field in the horizontal plane. As a result, there are two sets of closed magnetic field line loops or islands pressed to each other in equilibrium by the action of the magnetic field. This equilibrium is however unstable under small perturbations. In this case, the two islands rotate until reaching a horizontal position from which they are expelled in opposite directions under the magnetic field influence.

We will use the Strauss and Longcope model to determine the best way to add second order methods to M3D. On promising possibility is to add a hierarchical correction to the first-order methods currently in M3D. If so, this would greatly simplify the implementation and interaction of the first- and second-order terms in the discrete model.

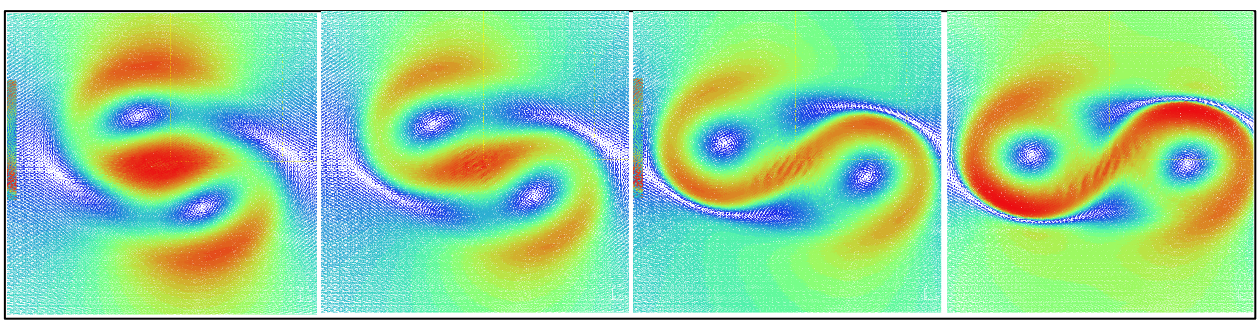


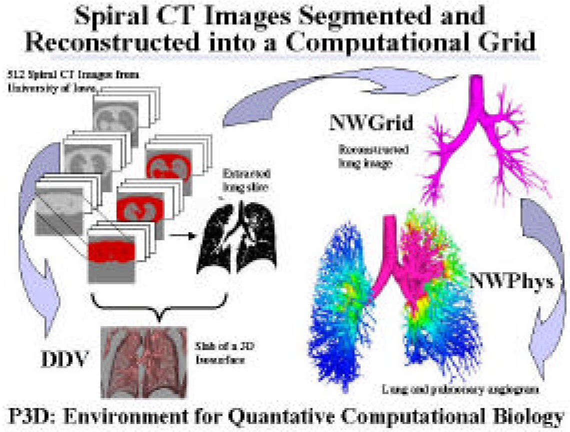
Figure 7 Tilt instability example

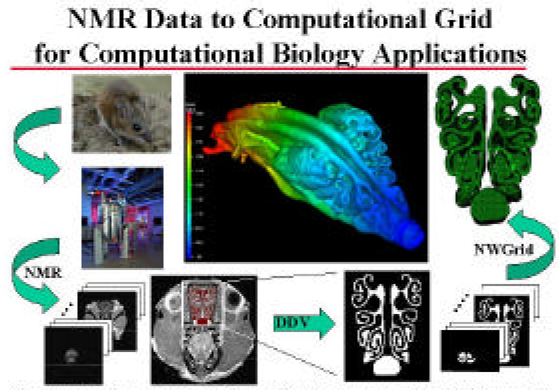
2.1.6 Biology

TSTT Personnel: Harold Trease (PNNL)

Biology Personnel:

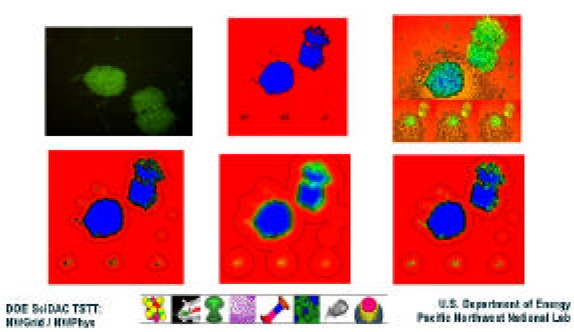
In addition to the five primary SciDAC application areas that the TSTT Center supports, we are also incorporating TSTT meshing and discretization capabilities into DOE-funded computational biology applications. This activity is designed to coordinate and cultivate a relationship between TSTT capabilities and DOE's biology areas. Specifically, this was done by incorporating TSTT (NWGrid/NWPhys) mesh technology and CCA-compliant component technology into two

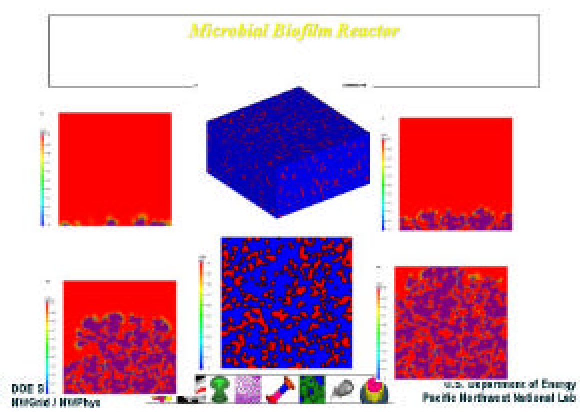




The upper respiratory tracts of 5 Sprague Dawley rats were successfully imaged by NMR and reconstructed using DDV and NWGrid.

ongoing DOE programmatic areas in Microbial Cell Biology (DOE LAB 01-20) and Computational Biology (DOE LAB 01-21). In addition, application support was provided to several internal PNNL LDRD projects that are directed toward multi-scale computational biology, like the Virtual Lung Project and Nano-biology projects. The main focus of these efforts is in image reconstruction and feature extraction of computational geometry and meshes representing complex biological systems that include everything from individual cells (procaryotic and eucaryotic) to organs (like lungs, upper respiratory systems, whole organisms). The figure on the left represents the process of extracting the meshed geometry of a lung and arterial branching tree from the volume image data for a CT scan of a human chest. The figure on the right represents the process of extracting the computational geometry and mesh for the upper respiratory tract of a rat based on volume NMR images. The following two figures are simulations of microbial cell communities (left) and microbial cell biofilms (right) using the TSTT NWGrid/NWPhys mesh generation and discretization codes. The figure on the left is of the diffusion of oxygen into a community of Shewanella bacteria (images are from confocal microscopy where the microbes have been stained using GFP. The figure on the right is the growth of a biofilm within a bioreactor (imaged using NMR).





2.2 Technology

The primary driver for our development of new technology is the creation of interoperable and interchangeable meshing and discretization components that can be used in terascale computing environments. Our efforts in FY02 fell into four broad categories.

- Development of technologies that aid interoperability directly such as the definition of a common mesh interface, the creation of CCA-compliant mesh components, and demonstrations of TSTT tool interoperability on a one-to-one basis (Section 2.2.1).

- Laying the groundwork for the development of the TSTT Discretization library by isolating the appropriate technologies from TSTT frameworks (Section 2.2.2).

- Creating a new mesh quality improvement toolkit that can be used with all TSTT technologies and that will be enhanced to support hybrid meshes (Section 2.2.3).

- Continuing to develop parallel and adaptive meshing algorithms that are appropriate for use on terascale computers (Section 2.2.4).

2.2.1 Interoperability

The bulk of our efforts toward the goal of interoperable meshing and discretization software in the first year has focused on the development of a common interface for mesh geometry and topology access, and we describe these efforts in Section 2.2.1.1. To ensure that our tools are as broadly available as possible, we have worked closely with the Common Component Architecture (CCA) forum to investigate the use of their SIDL/Babel language interoperability tools and to ensure that our interfaces will be compatible with the CCA component specification. This work is described in Section 2.2.1.2. Finally, to demonstrate the promise of interoperable tools, we have been working to merge two TSTT tools, Overture and Frontier, to create a powerful simulation tool that combines adaptive mesh refinement and front-tracking techniques, and we describe these efforts in Section 2.2.1.3.

2.2.1.1 Common Interface Definition

One of the primary development efforts that showcases TSTT teamwork is our creation of common interfaces for mesh geometry and topology access. Most of the TSTT sites have participated actively in this effort through face-to-face meetings, teleconference calls, and definition and implementation efforts. The work was initiated at a kickoff meeting held at Argonne on Sept 11-12, 2001, and we have worked since that time to define a basic set of interfaces for static mesh query and access

Our philosophy has been to focus primarily on the definition of accessor interfaces that provide the functionality needed by application programmers. A key aspect of this approach is that we do not enforce any particular data structure or implementation with our interfaces, only that certain questions about the mesh (such as geometry or first-order adjacency information) can be answered through calls to the interface. The challenges inherent in this type of effort include balancing performance of the interface with the flexibility needed to support a wide variety of mesh types and the desire to keep the interface minimal so that it is easy to implement and adopt.

As of September 2002, the TSTT interface definition group has agreed to nomenclature regarding mesh entities and basic functionality for accessing geometric and topological information about the mesh. In particular, the TSTT interface supports topologically-dimensioned entities which are called VERTEX, EDGE, FACE, and REGION for 0-3D respectively. Each of these entities can live in a geometric dimension equal to or greater than its topological dimension although we assume that the geometric dimension is the same for all entities in a given mesh. In addition, various topological regions are supported; in particular, TRIANGLE, QUADRILATERAL, and POLYGON are supported in 2D and TETRAHEDRON, HEXAHEDRON, PRISM, SEPTAHEDRON, and POLYHEDRON are supported in 3D. Access to the mesh geometry and topology information is provided through a number of different mechanisms. For example, care was taken to ensure that access to coordinate and adjacency information in the mesh was provided on both an entity-by-entity basis by using iterators of opaque objects and for the entire mesh at once through arrays of doubles. All implementations are required to support both modes of access although it is recognized that only one style is typically native to the underlying implementation thus may require a copy operation if the other mode of access is requested. To improve performance of the entity-based functions, a workset iterator interface is provided that allows the user to request entities in an array of a user-specified size (for example, 100 entities at a time). These arrays can then be used in any of the entity-based function calls to retrieve large chunks of information to minimize the number of calls through the interface. Additional functionality that is currently supported for the mesh includes mesh creation, loading, destruction and services to access basic information such as its geometric dimension, the number of each type of entity, etc. Finally, the user is able to attach an arbitrary piece of data to any mesh entity or to the mesh itself through the use of "tags". This allows the interface to become useful to application scientists by providing functionality for attaching boundary condition information, material properties, etc. In total, this interface contains 39 functions and provides the functionality needed to support a basic mesh-based simulation.

Implementations of this specification are underway at LLNL (for Overture), PNNL (for NWGrid), RPI (for AOMD), SNL (for MDB/CUBIT), and ANL (for a simple triangular mesh). Additional efforts that use the interface for interoperable meshing technologies are ongoing at SUNY SB as part of the Frontier merge with various TSTT mesh generation technologies and as part of the MESQUITE mesh quality improvement toolkit.

In addition to the basic interface specification described above, a number of additional functionalities have been discussed and the interface definition efforts for them are well underway. In particular, we are considering the addition of

- mesh sets that allow arbitrary groupings of mesh entities,

- submeshes that support the mechanisms needed in an interoperable meshing environment such as parent child relationships among meshes as well as data transfer among meshes,

- parallel queries to support distributed computing, mesh modification interfaces to support adaptivity, and

- fields and degrees of freedom managers to support the development of the TSTT discretization library.

Work has proceeded primarily through two face-to-face meetings of the interface definition group (September 11-12, 2001 and August 22, 2002), 2 hour teleconferences held approximately every three weeks, the use of electronic notebooks and an archived email discussion groups, as well as opportunistic meetings at conferences such as the 10th International Meshing Roundtable.

This work has been presented at a number of different workshops and conferences to audiences that are interested in a similar goal of common interface definition. In particular, we have interacted with participants in the NSF Adaptive Software Program ITR led by researchers at MSU and Cornell, with Sandia scientists who are hoping to develop data services interfaces, with participants in the unstructured grid generation forum who are developing interfaces for mesh generation routines (http://www.eps.gov/spg/USAF/AFMC/AFRLWRS/PRDA-VAK-02-06/listing.html), and with participants of the CMU mini-roundtable workshop held at the 11th International Meshing Roundtable Conference on common data structures/libraries for mesh generation particularly as it pertains to Delaunay tetrahedralizations (http://www.aladdin.cs.cmu.edu/workshops/meshing.html).

2.2.1.2 Use of CCA Technologies in the TSTT Interface Definition Efforts

Throughout the first year, the interface definition group has worked in conjunction with the Common Component Architecture (CCA) Forum in a number of ways to ensure that the TSTT interfaces are compatible with CCA specifications. Our efforts fall into two major categories.

First, we have done a significant amount of work to understand and use the Scientific Interface Definition Language (SIDL) and associated Babel compiler developed as part of the CCA effort. This work is motivated by the fact that many of the TSTT tools are written in C++ and most of our targeted applications are written in Fortran. We did not wish to settle for the "least common denominator" solution of using arrays for all of our data transfer. Thus we are using the SIDL tool to define our interfaces in a language independent manner and to facilitate the consistent and efficient implementation of language bindings to these interfaces. In particular, we have generated and used the C, C++ and Fortran bindings for various TSTT mesh implementations. In addition, LLNL has created a prototype interface for fields and operators using SIDL. To help all TSTT sites incorporate SIDL as part of their everyday work environment, Kyle Chand (LLNL) has developed a simple SIDL tutorial that incorporates a simplified version of the TSTT interface and has distributed this tutorial to TSTT researchers. Ongoing work is being performed to clearly understand the performance ramifications of using SIDL/Babel, particularly on fine-grained operations such as entity-by-entity access to mesh geometry and topology. In particular, we are investigating the possibility of providing language- or tool-specific access to the underlying meshes for the cases where high performance is critical for this type of access. Early efforts include a development of a C++ version of the TSTT interface that bypasses the SIDL intermediate object representation (written in C). However this work is very preliminary; much more needs to be done to evaluate the performance ramifications of SIDL on our interface and to develop solutions that are compatible with the SIDL specification (currently planned for year 2). Second we are developing TSTT and CCA-compliant mesh components and using them with other numerical components to demonstrate their ability to solve application problems. The first application involves a two-dimensional TSTT mesh that was used in conjunction with time integrator, linear solver, MxN redistribution, and visualization components (all developed at different labs as part of the CCA Forum efforts) to solve a time dependent PDE in the CCAFFIENE framework developed at SNL. This work was demonstrated at SC01 and continues to be used to illustrate complex application scenarios in the quarterly CCA tutorials. The second application was developed using the NWGrid meshing software from PNNL. In this case, a SIDL version of the TSTT interface was used to generate a Fortran binding for NWGrid so that it could be used with a mesh quality improvement component (based on Opt-MS algorithms from

ANL) that was written in C. These components were successfully deployed and used in the DeCaf framework developed by LLNL.

2.2.1.3 TSTT Tool Interoperability: FronTier and Overture

To showcase the potential payoff for an environment that supports interoperable meshing and discretization software, we have engaged in a few efforts that target one-to-one interoperability between TSTT tools. The most notable effort in this regard is the ongoing work to merge the FronTier front-tracking code with the Overture adaptive mesh management framework. FronTier (SUNY SB and BNL) has been used to apply the front-tracking method to different scientific problems such as gas dynamics, petroleum reservoir study, MHD and solid interface problems. Overture (LLNL) is a mesh management framework for problems involving complex geometry that uses Berger-Colella block-structured adaptive mesh refinement (AMR) to insert highly refined patches in regions where wave interaction demand increased resolution in the interior region. Our goal within the context of the TSTT center is to combine the strengths of the FronTier and Overture codes to develop a new, efficient front-tracking algorithm combined with the AMR technique, the so-called AMR Front Tracking Method.

This work was completed primarily at SUNY SB with help from the Overture team at LLNL, and through the last year, this project moved through three phases. The first phase involved a complete understanding of the Overture algorithms and its implementation. This included understanding its objectives, the implementation of the relevant algorithms, as well as its data structures, functions, and the computational environment.

The second phase involved resolving the conflicting definitions and macros in the two codes. Because the two codes were developed independently, a number of conflicting definitions, function names and macros with identical names were used for similar (but not exactly the same) or different purposes. These conflicts were resolved by restricting most of the necessary changes to the FronTier code, thereby ensuring easy access to future Overture upgrades.

In the third phase, our objective was to construct a common interface for the communication of data in the two codes. The most difficult part of the work has been in the generalization of patch and subdomain communications. Although FronTier is parallelized, the data communication between patches inside the same parallel processor is outside of the development framework. As a result, we needed to find a practical method to synchronize the computation of different patches inside the same parallel processor. We finally decided to modify the entire functional structure of the interface propagation in the FronTier code to have it fully modularized at the synchronization points inside a single driver function. Figure 8 shows the adaptive patches with the tracked front.

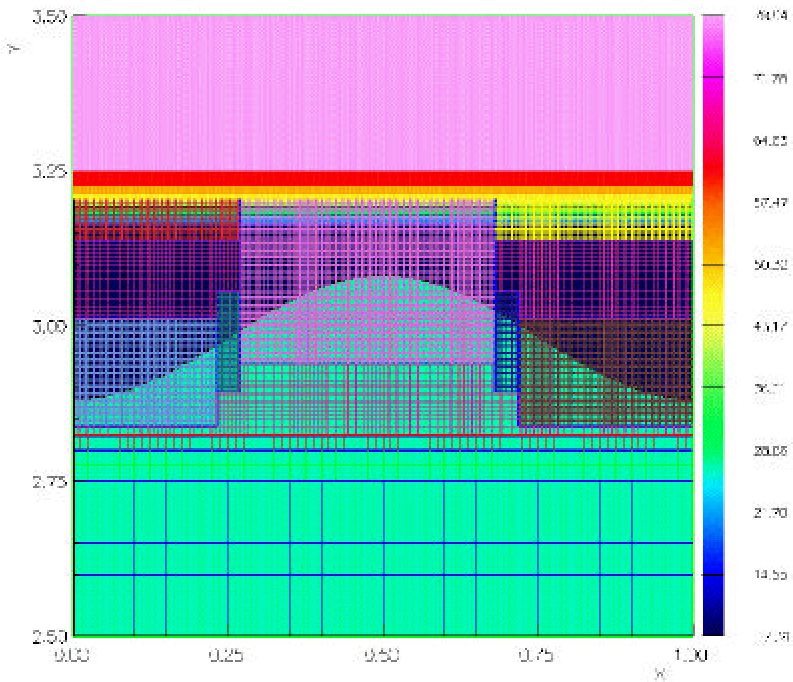


Figure 8 The adaptively refined patches and the tracked front in a combined Overture-FronTier initialization.

2.2.2 The Discretization Library

Efforts in FY02 have been primarily focused on creating the infrastructure necessary for the discretization library development. The TSTT center has a great deal of expertise in high order and adaptive discretization strategies, but most of the implementations are tightly coupled to existing TSTT frameworks and are not suitable for direct insertion into a stand-alone library. Thus a great deal of effort at LLNL, RPI, and ANL has gone into separating and re-implementing low level operators from their respective frameworks.

In particular, the LLNL team has focused on creating new, optimized versions of the Overture operators as Fortran-callable functions for structured grids which include both conservative and non-conservative difference approximations. The non-conservative operators are available to 2nd and 4th order. The addition of 4th order conservative approximations is under consideration. There are functions to evaluate the derivatives and also functions to form the sparse matrix corresponding to the operator. Most of the derivative operators are now completed and work has begun on some of the interpolation functions, such as those needed for AMR interpolation.

Simultaneously, efforts at RPI have focused on redesigning Trellis to increase its componentization. Trellis is now divided into four modules.

- A parallel mesh database, PAOMD, that provides critical capabilities for accessing the mesh, doing mesh adaptation and handling parallel mesh representations. The mesh database is independent of the other modules and can be distributed separately. PAOMD provides a TSTT mesh interface. Some extensions have been added to the mesh database: integration, curved elements and mapping, geometrical queries and searches in large meshes, parallel toolbox.

- A function space library that provides generic approximation schemes capabilities for finite-dimensional field families and contains the interpolation schemes (Lagrange, Szabo, Aiffa, Dubiner).

- A discretization library that provides basic differential and integral operators that act on the function spaces. Differential operators include standard operators such as Grad, Div and Curl and those commonly used by applications such as various strain definitions. In the application of weak forms (e.g., finite element, finite volume, partition of unity) local contribution to the global system of discrete equations are constructed through the appropriate integration of discrete entities (elements, element faces, etc.) of appropriate differential operators acting on weighting and trial spaces that are in terms of the selected members of the function space library. To support the definition of these contributions Trellis supports the effective construction of linear, bilinear, trilinear and a general operator. The discretization library also provides the important capability of managing degrees of freedom. Degrees of freedom (DOF's) are the coefficients of the function space members employed in the construction of the contributors. The DOF Manager is a purely algebraic tool that is able to store, retrieve, and delete DOF's.

- A Solver Driver that provides capabilities to solve multiphysics problems. The Solver Driver can interface to solvers such as PETSc, Sparskit or DASPK.

In addition, at ANL, Fischer has worked to separate the high-order spectral elements used in the Nek5000 framework. He has created a self-contained set of routines to general spectral discretrization components on an element-by-element basis. He currently supports a number of different operators commonly found in PDE simulations and is working to provide both Fortran and Matlab implementations.

Finally, preliminary efforts are underway to define the common interfaces needed for discretization operators and fields. An initial draft based on a prototype implementation was proposed by the LLNL team at the August 2002 interface definition meeting and was briefly discussed. More work in this area will continue and is a priority for the interface definition group in FY03.

2.2.3 MESQUITE Mesh Quality Improvement

It has long been known that achieving accurate and efficient numerical solutions to PDE-based applications depends essentially on mesh quality. To improve the meshes generated as part of the TSTT project, we are developing a mesh quality improvement toolkit called MESQUITE. The primary aim of this project is to provide a freely available, comprehensive software package that would accommodate a number of different mesh element types, quality metrics, and state-of-the-art topology modification and node point movement algorithms. Although we designed MESQUITE from the ground up in FY02, this toolkit is based on the mesh quality improvement algorithms and software developed previously at SNL and ANL.

At the end of the first year, MESQUITE development is well underway. We have assembled a team of five TSTT researchers including Michael Brewer (SNL), Lori Freitag (ANL), Thomas Leurent (ANL), Patrick Knupp (SNL), and Darryl Melander (SNL). A primary accomplishment in FY02 was the creation of the MESQUITE design; it is general purpose and easily extensible to support new research in mesh quality improvement. The diagram in Figure 9 shows our high-level design. The use of classes such as MeshQualityMetric, ObjectiveFunction, VertexMover, and InstructionQueue help us achieve an object-oriented, flexible design. Embedded within the various classes are member functions where the computationally intensive calculations take place. These member functions avoid objects, use pointers, arrays, and other low-level data structures to ensure that the computations are as efficient as possible.

Based on this design we have written version 0.5 of MESQUITE in C++. This version implements the major MESQUITE classes, various metrics and objective function templates, and several numerical optimization methods. In particular, MESQUITE currently does mesh untangling, element shape improvement, and Laplacian smoothing on local mesh patches consisting of either triangular, tetrahedral, quadrilateral, or hexahedral unstructured meshes. The prototype has a number of state-of-the-art algorithms for optimization-based node point movement including steepest descent, conjugate gradient, and active set solvers. In addition, considerable attention was given to the development of a flat mesh data structure for the internal representation of unstructured mesh data that is both highly efficient and convenient. To obtain our mesh data from the application, we use the TSTT common mesh interface specification, and are currently working to support two tools that have completed implementation of the TSTT interface, namely AOMD (RPI) and MDB (SNL). The initial implementation of version 0.5 will be completed by November 15, 2002.

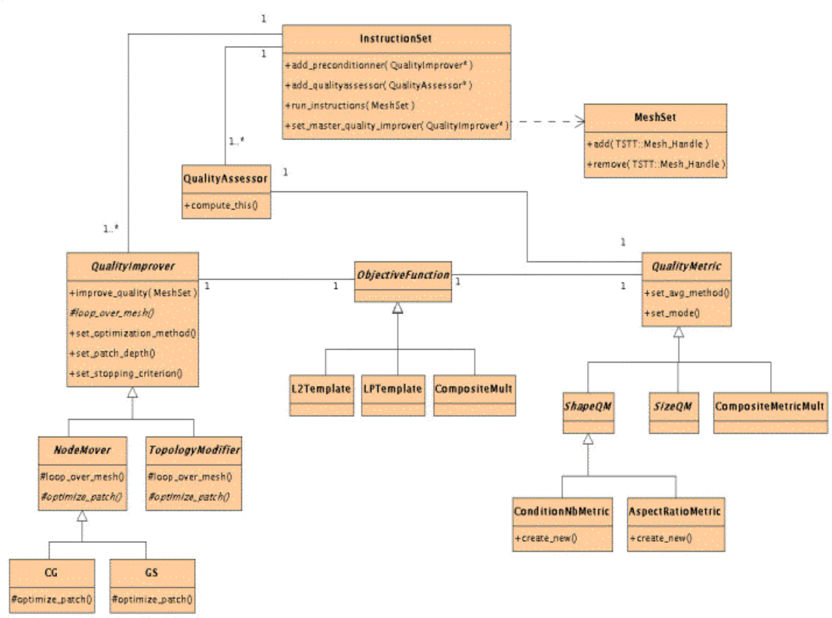


Figure 9 The MESQUITE design

2.2.4 High Performance Computing

The ability to support high-performance computing on distributed parallel computers requires the ability to distribute the mesh over the memories of these computers with complete knowledge of the interactions between the meshes on the various computers. To achieve this goal, information is typically maintained on each processor about the entities on its partition boundaries that it shares with other processors. This information is used to control the communication of information between the mesh partitions. The Parallel Algorithm Oriented Mesh Database (PAOMD) represents an extension to AOMD that supports these needs.

PAOMD maintains mesh information on the partition boundary similar to the information that must be maintained about mesh entities on the boundary of the domain. The key difference is that this information is supplemented with information indicating what processor the off processor neighbors are on along with the appropriate adjacency information. PAOMD provides the functions to build the messages needed for the interprocessor communications which are effectively supported using AUTOPACK from Argonne. To support adaptive computations PAOMD supports mesh migration and partition boundary updates; new partitions are determined by Zoltan (Sandia). PAOMD works with conforming and "matched non-conforming" mesh adaptations.

A second area of consideration is the relationship between distributed meshes and the implicit solution of algebraic equations on parallel computers, particularly in the case of adaptive computation where the mesh and the system of equations are in constant flux. As a first step toward investigation of this issue we have integrated PETSc into Trellis to provide it with an advanced set of equation solvers. The next step will be to consider, in collaboration with the TOPS ISIC methods for effectively coupling mesh partitions and equation systems defined from them with the goal of an effective coupling for adaptive calculations.

2.3 Interactions with ISICS

2.3.1 CCA

TSTT Point of Contact: L. Freitag

We have close collaborations with various members of the CCTTSS SciDAC center and have worked with them in a number of different ways to ensure that TSTT and CCA technologies will be compatible. In particular, Lori Freitag is a joint PI with the CCTTSS SciDAC center and has regularly attended the CCA quarterly meetings, jointly co-leads the CCA data subgroup with David Bernholdt, and helped organize a joint CCA/TSTT/APDEC meeting to initiate discussion of a common interface for block structured AMR packages to exchange data. For SC01, we worked with several members of CCTTSS to demonstrate the use of TSTT mesh components in the CCAFFIENE CCA-compliant framework to solve a time-dependent PDE. As mentioned in the meshing interoperability section, we are also working closely with SIDL and Babel to investigate the creation of language independent mesh components. Our basic interfaces are defined using SIDL, and additional work is now underway to determine the best way to provide high performance interfaces for entity-by-entity interactions.

Principal Meetings

- Quarterly CCA meetings (October 2001, Jan 2002, April 2002, June 2002)

- CCA/TSTT/Climate meetings to discuss the creation of interoperable interpolation components for the model coupling toolkit (ANL 2001-2002)

- CCA/TSTT/TOPS Meeting. December, 2001. Discussed the use of SIDL for the TSTT mesh interface, created a preliminary implementation.

- APDEC/CCA/TSTT open meeting. April 10, 2002. Discussed preliminary version of block structured AMR interfaces. FLASH scientists also attended.

2.3.2 TOPS

TSTT Point of Contact: M. Shephard

Initial interactions with TOPS have focused on a careful examination of the latest version of PETSc (a key TOPS solver technology) and its integration into Trellis. The integration into the new version of Trellis has been carried out for fixed mesh analysis using the Trellis DOF manager to coordinate the linkage with the overall global systems and to provide the assembler with the mesh entity level contributors. The contributors have been assembled into appropriate PETSc structures for solution. Initial parallel analyses are underway and efforts to ensure efficiency are beginning.

An examination of the issues surrounding the support of adaptive calculations has been started by determining which PETSc structures will best support such simulations. One natural selection is the matrix free GMRES method. We plan to investigate the application of the matrix free GMRES for an adaptive calculations. Efforts will then begin on the long-term effort with TOPS developers to determine the most effective methods to combine TSTT adaptive mesh structures with TOPS solvers.

In addition, we are carefully following the definition of the TOPS vector, matrix, and solver interfaces to ensure that the compatibility of our discretization library. These interfaces are still under development (primarily at ANL) and Freitag has attended several meetings with TOPS scientists to discuss their development as it relates to TSTT functionality.

Principal Meetings

- August 20-21, 2001. TOPS Kickoff Meeting. Shephard attending for TSTT. Presented an overview of the TSTT center to the TOPS researchers.

- Oct 26, 2001. Shephard and Freitag attending for TSTT, Smith attending for TOPS. Discussed the efficient integration of solver technology with adaptive mesh techniques.

- August 23, 2002, Argonne. Brief discussions with Barry Smith on adaptive analysis and PETSc.

2.3.3 PERC

TSTT Point of Contact: D. Quinlan

Current interactions between PERC and TSTT are focused on the expected support within the ROSE project for the TSTT Discretization Library. Current work is focused upon the use of ROSE to define transformations that optimize the use of mesh operators in C and C++ applications. This is closely related to the TSTT Discretization library which will also have numerous operators. Current work has demonstrated initial parts of this work using relatively simple operators and improved the performance by a factor of 4-6 on structured grid computations. The current work was presented in several papers published earlier this year. Since Dan Quinlan is a part of both ISICS (TSTT and PERC), and working on both the ROSE project and the TSTT Discretization Library, no official meetings have taken place or are required [sic. for Dan to talk to himself].

2.3.4 APDEC

TSTT Point of Contact: D. Brown

The *Center for An Algorithmic Software Framework for Partial Differential Equations* (APDEC) is developing a high-performance algorithmic and software framework for solving partial differential equations arising from problems in three important mission areas for the DOE Office of Science: magnetic fusion, accelerator design, and combustion. The core meshing technology being used by APDEC is adaptive mesh refinement (AMR) on embedded boundary (EB) meshes. EB meshes are Cartesian meshes in which boundaries are described by arbitrary cutting surfaces, resulting in partial cells near the boundary. The Overture project at LLNL contributes research and development activities to both TSTT and APDEC. In particular, the Overture project is responsible over the next few years for delivering a stand-alone capability for building geometry and EB meshes either from scratch, or starting with CAD geometry data. The EB mesh representations will be compatible with the meshing interfaces under development by TSTT, thus allowing interoperability with the other meshing technologies within TSTT. The EB mesh generator will also be available as part of the TSTT meshing technology distribution. LLNL staff meet regularly with members of the APDEC project at Lawrence Berkeley National Laboratory.

Principal Meetings:

- APDEC Technology Meeting. August 22, 2001. David Brown, Bill Henshaw, Kyle Chand, Anders Petersson attending for TSTT.

- Meeting with APDEC. Sept 25, 2001, Shephard and Flaherty attending for TSTT. Colella attending for APDEC.

- APDEC Kickoff Meeting. November 8-9, 2001. David Brown, Petri Fast attending for TSTT.

- APDEC –TSTT communication. Phil Colella (APDEC) and David Brown, Jim Glimm (TSTT). Jan. 15, 2002 and following email exchanges. Discussion of scientific issues associated with use of AMR in the POP ocean code.

- APDEC/CCA/TSTT open meeting. April 10, 2002. Discussed preliminary version of block structured AMR interfaces. FLASH scientists also attended.

3 FY03 Plans

The FY03 plans (with comments and comparison to the original proposal) are summarized in the table below and developed in detail in the remainder of this section. In general, we will continue to focus activities that will impact the SciDAC application areas identified with FY02, develop common interfaces for TSTT technologies, and showcase the promise of mesh and discretization interoperability through one-to-one integration efforts such as the FronTier-Overture merge. In addition, we will build on the low level interfaces defined in FY02 to deploy new technologies such as MESQUITE in all TSTT tools and to develop interfaces that address interactions with fields and discretization operators, CAD and image data geometry. We will also begin to focus on a hierarchical approach to the problem definition as described in the proposal which is necessary for a general solution to interoperable meshing and discretization.

3.1 Applications

We plan to continue to devote a significant portion of our resources to interactions with the SciDAC application teams. Our primary goal is to use TSTT technology to impact the application efforts either through direct insertion of TSTT software into the application solution process or through the development of new techniques and software for the application codes that use TSTT technology. Toward that end we will continue to work with scientists in accelerator design, astrophysics, climate, combustion, fusion, and biology.

3.1.1 Accelerator Design

LLNL will continue to investigate techniques for improving the discretization schemes used in Tau3P with the end goal of improving the robustness of that code. This will include the continued analysis and development of DSI-like methods for solving wave equations in general and Maxwell's equations in particular. The objective is to design schemes that are uniformly stable on many classes of meshes, including general non-orthogonal hexahedral meshes, tetrahedral meshes, and hybrid multi-element meshes that include hexahedral, tetrahedral and pyramidal cells. Such methods may involve the development of spatial filtering/dissipation techniques for the DSI method, or possibly the redesign of the discretization algorithms altogether. We will implement and test these methods using the Overture framework, and also develop approaches for stabilizing Tau3P as non-invasively as possible.

SNLA will also work on the improvement of meshes for Tau3P. The results of the study on correlations between Tau3P cutoff times and mesh properties will be used to determine how the meshes used by SLAC can be improved. For example, if minimum mesh edge length proves significant in determining cutoff time, then we will investigate automatic node movement strategies (smoothing) to increase this minimum length. Improvements to the meshes by smoothing (MESQUITE) or by new meshing algorithms in CUBIT or Overture will be investigated. It is hoped that improvements in the mesh such as this will directly increase the Tau3P cutoff time.

FY03 Proposal	FY03 Adjusted	Comments
Refine and complete definition of the low level interfaces and deploy them within the TSTT tools	Critical and should continue with high priority	
Preliminary definition of the interfaces for the common interfaces for the geometry (CAD and image) and physics attributes	This effort depends on the low level mesh interface and once that is complete, work will begin in this area.	
Preliminary work to define the problem hierarchy and interfaces necessary for hybrid methods	This is an important area that requires the completion of the low level interfaces. We will continue to pursue the work initiated in FY02.	Initiated FY02
Deploy the a priori mesh improvement tools into the TSTT mesh generation and management tools via the low level interfaces defined in FY01	This effort is on track an our initial efforts will be to integrate MESQUITE with Cubit and AOMD.	
Complete interface specifications for the discretization library; begin implementation of the low-level operators and interface them to TSTT mesh technologies; work with the appropriate ISICs to define interfaces for interacting with linear and nonlinear algebraic components	Change "Complete" to Contin ue… depends on completion of low level query interfaces	
Continued enhancements to the mesh generation capabilities	Eliminated due to budget constraints	
Initial work to merge front tracking algorithms with existing codes including TSTT tools such as Overture	"Initial" should change to continue; NWGrid should be investigated, year 1 deliverable FrontierLite will be investigated in FY03	
Begin implementation of the parallel decomposition (level 3) that uses information on the mesh hierarchy for effective parallel control	Depending on progress with related activities we will begin this effort this year.	
Consider how parallel mesh generation procedures will be extended to take full advantage of the hierarchic structures	Eliminated due to budget constraints	
Develop software design principles facilitating downstream use of hierarchical data structures	Make a preliminary assessment of how hierarchical information we generate may be exploited in downstream applications, focusing on iterative solver technology under development in related ISIC's – Tim Tautges will lead	
Insertion of initial parallel adaptive simulation technologies into the fusion (RPI), accelerator (BNL), climate (ANL) and biology (PNNL, ANL,SNL) applications	Deliver TSTT technologies to the application scientists in such a way that significant impact is had.. For example, adaptivity in SEAM and biology applications, mesh quality and discretization to SLAC, and discretization to Fusion and Astrophysics.	Insertion into fusion production code will be very challenging, accelerator work is not funded by TSTT, climate SEAM is a good possibility, Biology is likely. In general, parallel adaptive simulation is too particular; use TSTT technology instead.
Insertion of existing mesh generation and geometry capturing technologies for complex geometries in the biology and chemistry applications	On track	
Documentation of new libraries, development of comprehensive test suites and automatic testing facilities, release of existing codes via the web repository (these activities continue through FY05	This on track for the individual tool development efforts.	

The correlation study may be extended in several ways. First, if we are able to add an effective spatial filtering scheme into Tau3P, we can investigate the sensitivity of cutoff time to mesh properties when this new algorithm is used. Second, using error estimators, we can investigate correlations between simulation error and mesh properties to identify the most important mesh-related factors affecting accuracy. Third, we can investigate correlations between simulation runtime (efficiency) and mesh properties. Based on these results we can consider improvements to the SLAC meshes to improve both accuracy and efficiency.

Finally, we will continue to investigate ways in which TSTT can help SLAC analysts clean up their geometries and reduce the time it takes to create a mesh.

3.1.2 Astrophysics

In the astrophysics applications we will continue to explore high order, adaptive discretization strategies with both the TSI team at ORNL and the magnetic reconnection team at University of Chicago.

In particular, with the TSI team, we will test the DG method developed for radiation transport on increasingly difficult problems until the existing one-dimensional, in physical space, supernova model is solved. To this end the next problem to be studied will have no scattering at all but will include emission and absorption of radiation. Once this study is complete, we will examine a still harder problem that combines scattering, emission, and attenuation of radiation. Finally initial tests with a simplified model of coupled fluid flow and radiative transfer will be attempted. In addition, we will work closely with TSI to implement the 3D caching scheme (in phase space) for optimizing the computation of scattering kernels.

With University of Chicago, TSTT researchers at RPI will work to integrate the DG capabilities and local time stepping techniques developed at Rensselaer into the FLASH code. We note that our efforts in this area are covered by two projects. Under a renewal of the ASCI FLASH center, we plan to study the effectiveness of DG methods on non-conforming, adaptive, Cartesian meshes. Under the TSTT project, we will investigate two areas. The first is the possibility of providing a linkage between the FLASH code and the TSTT mesh interface. The second will be to investigate the effectiveness of using the anisotropic mesh adaptation capabilities of Trellis to solve some of the same problems being addressed in FLASH on Cartesian grids. The first goal of this aspect of the project is to determine the classes of problem for which each of the approaches is superior. If it is demonstrated that there are relative advantages of the two methods for different problems, future (e.g., FY04) efforts could consider the possibility of using TSTT technologies to allow the use of the better of the approaches given the same overall problem specification.

3.1.3 Climate

We will continue to expand our existing activities with the climate SciDAC centers at ORNL and NCAR in FY03 and in addition, we will initiate a new activity on mesh quality improvement with the group at Colorado State University.

In particular, with ORNL climate scientists we will work to extend the grid refocusing techniques to unstructured hybrid meshes, e.g., geodesic icosahedra meshes on spherical geometries. We also intend to incorporate more of the climate physical variables and parameters into the mesh adaptation process. PDE-based smooth quasi-conformal mapping is used to produce the adapted meshes. This will lead to better prediction of climate simulation via mesh/grid refocusing and adaptation. For example, mesh refocusing can be used to obtain higher resolutions over the Rocky

Mountains. This would lead to better predictions of the long-term rainfall over the Northwest that has major effects on agriculture and wild fires. In addition, adapted moving meshes are possible to track special weather features like hurricanes. Another application is using stretched meshes to resolve scales and processes associated with topography where the mesh is focused over high altitude mountains.

With NCAR scientists, TSTT researchers at ANL will extend their conforming spectral element discretizations to support localized, nonconforming, quad-tree refinement because it is clear that the intermittent nature of the quantities of interest in climate simulation will benefit from a lightweight adaptive meshing strategy. We have contacted the AOMD group at RPI and the SPECULOOS group at EPFL, Lausanne, to investigate commonalities in current object-oriented approaches to high-order adaptive discretizations in large-scale parallel environments, and will use this knowledge to help define the TSTT interface for high-order discretizations.

Finally, a collaboration between TSTT and the Colorado State Climate SciDAC is planned for the beginning of FY03. The collaboration will investigate the effect of mesh quality on solution accuracy. The CSU group uses regular geodesic meshes on a sphere (hexagonal and pentagonal elements). The meshes are not completely regular, resulting in a non-smooth distribution of element area and edge lengths. The MESQUITE code will be used to create meshes with smoother distributions. Results of climate calculations using these smoothed meshes will be compared to the original climate calculations to determine if mesh smoothness (or lack thereof) has a significant impact on accuracy.

3.1.4 Combustion

We will use the AMR capability provided by the merged FronTier/Overture code that will be available in early FY03 to perform simulations of enhanced resolution. The goal of the simulations will be:

- to achieve a proper form of boundary conditions relative to grid resolution in the nozzle,
- to allow development of turbulent flow and improved resolution of pressure transients in the nozzle,
- to obtain quantitative agreement between simulation and measured velocities,
- to reduce uncertainty in inputs: pressure rise time and diesel viscosity, and
- to improve entrainment rates and comparison of simulation to experiment.

3.1.5 Fusion

Our primary efforts in this area will be to determine the most suitable form of *h-p* adaptivity for the applications of interest. The development of *h*-adaptive adaptive simulation techniques can be carried out with the current operational formulation. Two forms of *h*-adaptivity can be considered: non-conforming mesh refinement used in conjunction with DG formulations and a new conforming anisotropic mesh adaptation. A key aspect of the development of an anisotropic mesh adaptation procedure is the determination of an appropriate anisotropic mesh size field correction indicator.

However, in our investigations of the different problem formulations, we learned that the current stabilization of the stream function formulation works well for low-order spatial discretizations, but is not yet fully satisfactory for the general high-order discretizations needed for *p*-version adaptive methods. Efforts to address this issue building on results from stabilized finite element formulations will be carried out. Some recent results of T. Tezduyar that consider the relative contributions of the various stabilization terms by examining the appropriate matrix norms should be useful in this effort. In addition, consideration will be given to the most effective staggering strategies for solving the coupled equation systems.

Once effective high-order stabilization has been developed, consideration of *h*- and *p*-adaptivity can be initiated. Once these capabilities have been demonstrated, we will work with PPPL to determine how to get the appropriate set of these capabilities into codes they apply to their applications.

3.1.6 Biology

The plan for FY03 is to continue to support the DOE funded projects (LAB 01-20, The Microbial Cell Project and LAB 01-21, Computational Frameworks for Biology) by providing TSTT meshing and discretization capability for building a computational biology application framework called "The Virtual Microbial Cell Simulator (VMCS)". The VMCS is intended to provide mesh based image processing, image reconstruction, and simulation capability to ongoing biology programs (such as LAB 01/20-21) and to be incorporated into new ones such as the new DOE Genomes-to-Life (GTL) biology program and the DOE's response to Japan's Earth Simulator. The basic premise of this work is to provide multi-scale, mesh-based support for a computational biology applications that spans four levels of microbial cell biology (single cells, communities, biofilms, and populations). The TSTT Center can provide unique meshing and discretization capability to these programs.

3.2 Technology

We will continue to devote a significant portion of our resources toward our long-term goals of mesh and discretization interchangeablity and interoperability. First, we will continue to work as a team to define common interfaces for mesh and discretization and will build on the interfaces developed in FY02. Our focus will shift to mesh modification, discretization fields and operators, parallel query and mesh interoperability (see Section 3.2.1). We will also increase the level of effort devoted to the development of the Discretization library. This work required the completion of the low level interfaces for mesh access, and now that that work is nearly complete we can make more rapid forward progress on this aspect of TSTT (see Section 3.2.2). In Section 3.2.3, we will describe our plans for MESQUITE development including our planned interactions with TSTT tools and SciDAC application centers. Finally, in Section 3.2.4 we will discuss our plans for progress in the area of terascale adaptive algorithms.

3.2.1 Interoperability

In FY02 we have made good progress toward the development of interfaces that allow meshes to be interchanged within an application. To push forward, we have set the highest priorities for FY03 to be the following:

- Interfaces to support mesh modification. In particular, it is critical to define interfaces for element addition and deletion to support adaptive refinement algorithms, topology modifications, and mesh generation. Furthermore, interfaces that support node point movement are critical to the use of MESQUITE with TSTT tools.

- Interfaces that support access to a mesh distributed across the processors of a parallel computer. Mechanisms that allow the migration of mesh entities from one processor to another and that accept processor assignments for load balancing are critical and will be considered first. Initial efforts to provide general load balancing support will be accomplished by creating interfaces that are compatible with the Zoltan dynamic load balancing tool developed at SNL. Some TSTT sites use this tool already and work is being done in the CCTTSS center to create a Zoltan component. Options that support both entity-based messaging (for ease of use) and agglomerated messaging (for convenience) will be explored. We note that entity-based operations can be made more efficient by providing an optional interface to tools such as the AUTOPACK library developed at ANL, and we will investigate providing generic access to this tool to all TSTT meshes.

- Interfaces to support interoperability among meshes. In particular, we must consider the ramifications on our interface of allowing two or more TSTT implementations to coexist in one application. This work must be driven by applications and technology that require the use of hybrid meshes. We are currently working to identify such examples and have a number of promising technology motivators. For example, MESQUITE for hybrid mesh smoothing algorithms and the interoperability of Frontier with various TSTT mesh generation schemes. We are also working toward use of our interoperable meshing techniques in SciDAC application areas. The most promising example is the SLAC accelerator project which would like a combination of a nearly orthogonal grid near the center of the beam line with a high quality unstructured mesh near the waveguides and other areas of complex geometry.

In addition to the definition of core interfaces for TSTT mesh management tools, we must focus on the development of a discretization library that uses the TSTT interfaces. Preliminary work has been done to separate various discrete operators from large TSTT frameworks such as Overture (LLNL), Trellis (RPI), and Nek5000 (ANL). Initial discussions have begun for the creation of a common interface for accessing the discrete fields (or degrees of freedom) as well as for higher level operators and work in FY03 will proceed to complete these interfaces. Testing for compatibility with the low level TSTT query interfaces will ensure good performance and interoperability among tools. A proof of principle implementation will be targeted for completion in FY03 and initial discretizations will include finite difference, finite volume, finite element and discontinuous galerkin techniques. Later implementations will also include spectral elements and specialized finite elements such as the Whitney elements. Boundary conditions included in the first implementation will include Dirichlet and Neumann conditions. More sophisticated boundary conditions and user extensible options will be included in later years. The development of this library will be done with the TOPS matrix, vector and solver interfaces in mind as the two must be closely matched to obtain good performance in SciDAC applications.

We will continue our strong interactions with the CCTTSS center. In particular we will continue to explore the use of SIDL/Babel for providing language interoperability and will provide any feedback we have on generating high performance interfaces that are compatible with SIDL generated files to the Livermore team. In addition, we will provide TSTT mesh components to CCTTSS researchers and ensure that related numerical components that are developed (such as partitioners and solvers) are aware of and can successfully utilize the TSTT interface.

The work to demonstrate the power of TSTT tool interoperability through the one-to-one Frontier/Overture merge will continue. In FY03 we will unify the patch and subdomain communication, standardize a data interface between Overture and FronTier, and then fully test the combined code. We will test memory and CPU performance of the new code and its scientific performance in application problems. Once the 2D version is complete and well-tested, we will focus our efforts to the extension to three dimensions. We intend to distribute this new code combining AMR and front tracking algorithms to national laboratories such as the Argonne National Laboratory and the Los Alamos National Laboratory. We will also release this code to the authors of the Overture code for their evaluation and testing. We will modify the merger according to their expert opinion.

After successfully merging FronTier and Overture, we will begin a new phase of the research by studying the application of front tracking to biology applications in cell dynamics. This work will be in collaboration with Harold Trease (PNNL) and will use the standardized TSTT interfaces to accomplish the merge of FronTier with NWGrid.

3.2.2 Discretization

During FY03, LLNL, SNLA and RPI will lead the effort to complete specifications for a high level common interface and a low level interface to discretization operators and fields on TSTT meshes. Implementations of this interface will begin and continue into FY04. The high level interface is defined using SIDL/BABEL and will be used in a CCA-compliant component. The low level interface is more limited, and will be callable from Fortran application codes.

We will work with the TOPS SciDAC center and leverage their matrix and vector interface in the TSTT discretization library. Recent developments in PETSc will allow more efficient sharing of data and parallel data distribution by the linear solver libraries from TOPS and discretization operators from TSTT.

Each group within TSTT will implement an initial version of a subset of the discretization operators and fields while the interface definition effort is in progress. The initial target is to design and implement, in each group, a minimal Field object which can be used with a limited set of discretization operators: Laplacian, advection operator, and the gradient. Dirichlet boundary conditions will be implemented in this first pass. This version of the discretization library will be tested by solving a simple time dependent PDE evolution problem, such as the heat equation. The sample application developed by each group will access the computational grids through the TSTT mesh interface, and will demonstrate interoperability of the different mesh libraries: discretization operators from one application group can be used on a mesh from another group when accessed through the TSTT mesh interface.

The LLNL efforts will focus on the support of multi-physics simulations on sets of structured meshes, and on hybrid mixed element meshes in which most of the mesh is structured. The discretization library will be based on the Overture discretization library, which takes advantage of the large regions of structure to provide optimized computations of derivatives and matrix elements for implicit solvers. Second and fourth order difference approximations, including some conservative operators, will be supported.

The RPI efforts will focus on the support of multi-physics simulations on general unstructured meshes. Key areas to be emphasized will be the discretization library, solver driver and fields. Efforts on the discretization library will focus on supporting the effective construction of system contributors for weak forms by providing effective generalized operators. In addition to the basic linear, bilinear and trilinear forms, the ability to handle more general forms, stabilization operators, and error estimates must be considered and methods to support them developed. The solver driver efforts will consider how to most effectively control the interactions between the geometric discretization (the mesh), the local discrete parameters of the contributors, and the degrees of freedom of the global systems from which the solvers operate. RPI efforts related to fields will be focused on the proper handling of the solution parameter fields defined over the meshes, the operators needed to update those fields as the mesh is adapted, and the transfer of solution fields between meshes in multiphysics analysis. Specific procedures will be developed for the efficient local transfer of solution fields as incremental mesh modification operations are performed during an adaptive analysis. Methods that provide a single, efficient technique to map solution fields between two different meshes based on projection operations will be developed.

3.2.3 MESQUITE Mesh Quality Improvement

We plan to significantly expand the capabilities in MESQUITE to include new solvers such as the Feasible Newton solver developed by Munson (TOPS-ANL), a general simplex solver, the ability to perform global smoothing (to adjust all vertices simultaneously) and patch-based smoothing (to adjust some subset of the vertices simultaneously), the ability to smooth non-planar surface meshes, and to perform mesh quality assessment, and swapping on simplicial meshes. New mesh improvement criteria will include a surface orthogonality smoother, weighted smoothing, mesh alignment, and boundary-skew smoothing. In addition, we will work closely with application scientists in the SLAC and climate projects to develop mesh improvement strategies that are suitable for their particular needs. We will continue to work with the TSTT mesh generation tool providers and complete testing with the AOMD and MDB meshing tools. In addition, we will ensure that Overture and NWgrid technologies can take advantage of MESQUITE algorithms through the TSTT interface. We will create a users' manual and software documentation in preparation for releasing MESQUITE into the public domain which is currently planned for late spring 2003

In particular, for FY03, MESQUITE has the following goals which were derived, in the main, from discussions with numerical applications groups, both SciDAC and non-SciDAC:

Version 1.0 (Estimated April 2003)

- Install Feasible Newton Solver for faster optimization,
- Install Simplex Solver for mesh untangling,
- Add Global Patch smoothing for faster quality improvement,
- Add algorithms for smoothing non-planar surfaces,
- Enhance mesh quality assessment capability,
- Write initial Users' manual and documentation,
- Create an automatic regression test suite,
- Link MESQUITE to CUBIT and Overture codes,
- Smooth Colorado State geodesic meshes to improve accuracy,

- Smooth Accelerator meshes to improve stability, accuracy, and efficiency

Version 1.1 (Estimated October 2003)

- Add triangle and tetrahedron swapping capability,
- Add a surface orthogonality smoother,
- Add weighted smoothing for mesh copying,
- Add mesh-alignment smoothing,
- Add mesh boundary-skew smoothing,
- Add a mesh validity checking routine,
- Link to a mesh partitioning code to do non-local patch smoothing
- Add additional element types (pyramids, wedges) as needed,
- Update Users Manual,
- Link MESQUITE to NWGrid and use.

This set of goals is ambitious and may spill over into FY04. Further enhancements to MESQUITE will be prioritized according to the needs of SciDAC applications groups and then later by other customers.

3.2.4 High Performance Computing

The work in this area at RPI will continue and will focus on further development of the PAOMD tool. The initial version of PAOMD supports a limited set of geometric and equation discretization methods and structures. Efforts are required to extend the PAOMD methods to a more complete set. A first step in that direction will be the support of general mesh entity DOF sets with variable weights as needed to support various formulations including mixed variable and mixed order. A more complete set of mesh modification operations, including curved domain mesh geometric approximation improvements must be supported. One specific demonstration planned for the coming year is the use of PAOMD with conforming mesh adaptation including examples with a new SCOREC developed anisotropic mesh modification procedure.

Efforts will also begin on the consideration of the PAOMD mesh partitions with the TSTT mesh hierarchy. The TSTT mesh hierarchy will assume the existence of a high level definition of the domain and physical parameters associated with the simulation. A common option for the domain portion of this will be a non-manifold topological model which can be provided by a solid model, or extracted from an attributed mesh. One strategy to be demonstrated is to treat the PAOMD partitions as modifiers of that topological representation for the purpose of accounting for the partition boundaries. In addition to knowing that specific mesh entity classifications are defined only for the purpose of the partition boundaries, the ability to know which processor the appropriate entity "uses" are on must be effectively handled to meet the needs of interprocessor communication and partition updating as dictated by dynamic load balancing during adaptive analyses.

4 Interaction Lists

4.1 Interaction with Application Groups

1. January 15-16, 2002. SciDAC PI meeting. Brown, D Azevedo, Freitag, Glimm attending for TSTT. Presented overview of the TSTT center and interacted with a number of application groups about potential interactions.

4.1.1 Accelerator

2. Snowmass Conference on Accelerators, July 6, 2001, L. Freitag attending.: Presented an overview of the TSTT center to conference attendees, many of whom are involved in the accelerator SciDAC center.

3. August 23, 2001. Brown, Knupp, Samulyak, Henshaw, Quinlan, Chand attending for TSTT, Folwell, Ryne, Ko, and others attending for accelerator. Discussed the use of mesh quality metrics to diagnose problems with accelerator application. Also discussed use of Overture hybrid meshes in accelerator geometries. Progress to date. TSTT quality metrics are incoporated into the accelerator application for diagnostic purposes. Overture has meshed a trispal geometry with overlapping grids, is close to doing so with hybrid grids.

4. Meeting with Accelerator group. Roman Samulyak, Jim Glimm, Jim Davenport attending for TSTT. Robert Ryne attending for Accelerators. TSTT.

5. Oct 29--31, 2001. Discussed methods and their numerical implementation for modeling the particle beam electromagnetic wake field interaction and the use of TSTT technologies in the corresponding software modules.

6. Nov 14, 2001. Samulyak attending for TSTT. Ryne, Panagiotis, Spentzouris. Discussed load balancing issues in accelerator codes and technologies for modeling the 3D space charge problem and particle beam – electromagnetic interactions.

7. April 15, 2002. TSTT and SLAC Accelerator Meeting. Nate Folwell visited RPI to discuss mesh adaptation tools for unstructured meshes.

8. July 31, 2002. SLAC, Stanford CA. Brown, Knupp, Henshaw, Chand, Quinlan attending for TSTT. Ko, Folwell, ur-Rahman-Malik, Ng, Lixun Ge, Guetz and others attending for SLAC. Discussed mesh quality issues, geometry repair and cleanup, and stability issues with the DSI scheme used in SLAC’s tau3p code.

4.1.2 Astrophysics

9. Sept 6, 2001. Ed D'Azevedo, Ahmed Khamayseh, Valmor de Almeida attending for TSTT. Tony Mezzacappa, Bronson Messer attending for Astrophysics. Discussed the use of adaptive quadrature for astrophysics applications. Progress to date: Such procedures have been delivered to the astrophysicists. The astrophysics application is under modiffication by Bronson Messer to accomodate the adaptive quadrature formulation.

10. Oct 11, 2001. Freitag attending for TSTT. Rosner and Linde attending for astrophysics. Discussed the potential use of TSTT interoperable, multiple mesh technologies to support astrophysics applications.

11. Jan 14, 2002. Met with FLASH and IBEAM scientists at NASA Goddard to discuss the use of TSTT interfaces and CCA component technology in astrophysics applications.

12. February 7, 2002. TSTT and Astrophysics Meeting, Joe Flaherty, Jean-Francois Remacle, Lori Freitag, Ray Loy and Mark Shephard met with Bob Rosner's group to discuss the relationship of the discontinuous Galerkin (DG) developments and TSTT.

13. February 16-17, 2002. TSI Dallas Meeting D'Azevedo attending. Presented an overview of TSTT technology and discussed current/potential interactions with TSI group.

14. Frequent informal meetings between TSTT PIs and TSI PIs at ORNL to discuss ongoing work.

4.1.3 Climate

15. Nov 6, 2001, ANL Climate/CCA/TSTT Meeting, Freitag attending for TSTT; McInnes, Benson, Norris attending for CCA, Larson, Jacob attending for Climate. Discussed development of a CCA-compliant SCRIP tool that could use TSTT technology for expanding the capabilities to 3D.

16. Nov 15, 2001. NCAR Climate/CCA/TSTT Meeting. Freitag attending for TSTT. Drake, Larson, Jones, DeLucca attending for climate. Bernholdt, Rasmussen attending for CCA/ Discussed the development of a CCA compliant SCRIP tool with Philip Jones (the author) that uses TSTT technologies for various aspects such as 3D interpolation and vector interpolation.

17. August 6, 2001. Meeting with Ocean Modeling group. David Brown, James Glimm attending for TSTT, Robert Malone, Rick Smith, Phil Jones, and Rainer Bleck attending for climate. Plans formulated for insertion of local mesh refinement into POP.

18. February, 2002. Henry Tufo and Paul Fischer spent several weeks at NCAR to work with Steve Thomas and Richard Loft on filters and FEM-based preconditioners for spectral element methods. During that time, we also met with Annick Pouquet and Duane Rosenberg in the geophysical turbulence program to discuss avenues for development of adaptive spectral element codes.

19. Henry Tufo also spent several weeks during the summer at NCAR and, as of 9/1/02, has taken a half-time position there (the other half is at UC Boulder).

20. June 14, 2002. Climate SciDAC (CSU)/TSTT Joint Meeting, at Los Alamos National Laboratory, Todd Ringler, Patrick Knupp. Discussed the used of Mesquite mesh quality improvement algorithms in the climate application.

21. August 2002. Paul Fischer met with Steve Thomas (NCAR) at the Toronto workshop to discuss their work in climate modeling using spectral elements.

22. August 21, 2002. ANL Cimate/CCA/TSTT Meeting. Freitag and Curfman met with Larson and Ong to discuss progress toward the use of interoperable interpolation tools via TSTT and CCA technologies.

23. August 23, 2002. Meeting with Khameyseh and Larson/Jacob. Discussed the used of ORNL interpolation tools with the model coupling toolkit.

24. Frequent informal meetings between TSTT PIs and Climate PIs at ORNL to discuss ongoing work

4.1.4 Combustion

25. Combustion (J. Glimm, X. Li, A. Marchese, W. Oh, M. Kim (TSTT) and C. Tzanos (ANL)) Multiple email and phone conversations per week. Detailed discussion of technical progress and requirements.

4.1.5 Fusion

26. July 31, 2001. CEMM (Fusion) Kickoff Meeting. Tim Tautges attending. Presented an overview of the TSTT center CEMM researchers expressed an interest in field-aligned 2d tri meshes, possibly smoothing and solvers

27. August 6, 2001. Shephard, Flaherty, Remacle attending for TSTT, Jardin, Strass and others attending for Fusion. Discussed the use of high order methods and adaptive techniques in the parM3D code.

28. January 14-16 2002. TSTT and Fusion Meeting. Katia Pinchedez and Jean-Francois Remacle visited with Steve Jardin, Hank Strauss (NYU) and others at the Princeton Plasma Physics Laboratory to discuss the implementation of high order methods in the M3D code. During this visit, the main features of the M3D code were presented and a discussion took place to better define the goals of the PPPL team in terms of adaptive hp finite elements, and to determine the work to be done.

29. PPPM Hank Strauss (PPPM) and Roman Samulyak (TSTT) attending. Discussed use of FronTier to simulate the edge of plasma in MDH simulation.

30. May 13, 2002: PPPM (J. Glimm (TSTT) and Hank Strauss (PPPM)) Discussed progress of the TSTT-PPPM collaboration on higher order elements.

31. PPPM (R. Samulyak (TSTT) and H. Strauss (PPPM) Discussed use of FronTier to simulate edge of plasma in an MHD simulation.

32. July 8-12, 2002. Joe Flaherty and Jin Chen met during the SIAM National meeting in Philadelphia to discuss plasma fusion methods and discretization technologies. They each presented lectures on the RPI-PPPL interaction.

4.2 Interaction with ISICs

4.2.1 CCA

33. Oct 1, 2001. CCA Data Subgroup Meeting. Tautges, Freitag attending for TSTT. Allan, Bernholdt, Kohl, Freitag, Bramley attending for CCA. Obtained feedback on the first TSTT interface specification from the CCA data subgroup. To discuss combining these two groups for future interface development work. Progress to date: Recommendations for improvements in the TSTT interface specification were identified. A TSTT mesh component that is CCA-compliant was created and demonstrated at SC01.

34. Freitag regularly attends quarterly CCA meetings. Hosted the June CCA meeting at ANL and several TSTT members participated.

35. April 10, 2002. APDEC/CCA/TSTT open meeting. Freitag, Quinlan attending for TSTT. Discussed preliminary version of block structured AMR interfaces. FLASH scientists also attended (Also listed under APDEC).

4.2.2 TOPS

36. August 20-21, 2001. TOPS Kickoff Meeting. Shephard attending for TSTT. Presented an overview of the TSTT center to the TOPS researchers

37. Oct 26, 2001. Shephard and Freitag attending for TSTT, Smith attending for TOPS. Discussed the efficient integration of solver technology with adaptive mesh techniques

38. Aug 14, 2002. Freitag met with Smith, Knepley to discuss preliminary version of TOPS interfaces for vectors and matrices.

39. Aug 22, 2002. Smith and Knepley met with the TSTT interface definition group to discuss requirements for vector, matrix, and solver interfaces.

40. Sept 24, 2002 Glimm met with Keys at BNL and discussed use of TOPS in applications with reference to coordination with TSTT application efforts

4.2.3 PERC

41. July 17, 2001. PERC Kickoff Meeting. Dan Quinlan attending.

4.2.4 APDEC

42. August 22, 2001. APDEC Technology Meeting. David Brown, Bill Henshaw, Kyle Chand, Anders Petersson attending for TSTT.

43. Sept 25, 2001, Shephard and Flaherty attending for TSTT. Colella attending for APDEC. Discussed potential areas of interaction

44. November 8-9, 2001. APDEC Kickoff Meeting. David Brown, Petri Fast attending for TSTT.

45. Jan. 15, 2002. APDEC –TSTT communication. Phil Colella (APDEC) and David Brown, Jim Glimm (TSTT) and following email exchanges. Discussion of scientific issues associated with use of AMR in the POP ocean code.

46. April 10, 2002. APDEC/CCA/TSTT open meeting. Discussed preliminary version of block structured AMR interfaces. FLASH scientists also attended.

4.3 Related External Interactions

4.3.1 Astrophysics

47. Astrophysics (J. Glimm (TSTT), D. Sharp and B. Wilde (LANL)) February 24, 2002: Formulation of a test problem to show advantages of front tracking. Aug 14, 2002: Review of technical work on this test problem. Discussions of plan to write a paper.

48. Astrophysics (J. Glimm, Y. Zhang (TSTT) and P. Drake (U. Mich)) February 24, 2002 and multiple following email exchanges: Discussed plans to simulate nova experiments related to supernova explosions.

49. Astrophysics (J. Glimm, W. Oh, Y. Zhang (TSTT) and S. Woosley (UCSC))]January 15, 2002 and following email February 15, 2002: Discussed detailed initial conditions needed for simulation of supernova explosions.

4.3.2 Biology

50. Genomes-To-Life Applied Mathematics planning meeting sponsored by DOE MICS/OBER, March 2002, Washington, D.C.

51. Genomes-To-Life Imaging Technology planning meeting sponsored by DOE/OBER, April 2002.

4.3.3 Flow in porous media

52. Chevron (J. Glimm (TSTT) and Chevron personnel) May 29, 2001: Discussed Chevron plans for development of a new simulation code and the relations of this code to TSTT activities

4.4 Interactions within TSTT

53. July 12, 2001, TSTT Kickoff Meeting, Full TSTT ISIC attending. Also attending were John Drake (Climate) and David Keyes (TOPS).

54. Nov. 12, 2001. TSTT Technical Meeting. Representatives from each TSTT site attending.

55. TSTT Management Conference Calls. Most Friday afternoons at 5 pm eastern. Glimm, Brown and Freitag participating.

56. TSTT PI conference calls monthly. PIs from each site participating.

57. July 31, Nov 12. TSTT Management Meetings. Glimm, Brown, Freitag attending.

58. Sept. 11-12, 2001. TSTT Mesh Interface Working Group. Meshing and Discretization subgroups (approx 17 TSTT members). Discussed the interfaces needed for low level mesh query access. Progress to date: the first draft of the TSTT Mesh Query interface is created and implemented.

59. Oct 8, 2001. TSTT Mesh Interface Working Group at the 10th International Meshing Roundtable. Meshing and Discretization subgroups attending (approx 10 TSTT members). Recommendations from the CCA meeting were discussed and several were identified. Work is underway to create the 2nd draft of the TSTT interface specification.

60. TSTT Interface Definition group teleconferences about every 3 weeks.

61. January 2002, May 2002, August 2002, September 2002 Mesquite Meetings between ANL and SNL to plan and design the MESQUITE mesh quality improvement toolkit.

62. June 5, 2002 TSTT "Some-hands" meeting at the 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, Hawaii.

63. August 22, 2002. TSTT Mesh Interface Working Group. Completed the basic query interface and began discussion of fields and discretization.

64. August 23, 2002. TSTT All Hands Meeting. Assembled the TSTT team to discuss our status after one year of work. Presentations were given by each site and a determination of year 2 deliverables was made.

5 TSTT Publications

1. Adjerid, S., Devine, K.D., Flaherty, J.E. and Krivodonova, L. “A posteriori error estimation for discontinuous Galerkin solutions of hyperbolic problems,” Computer Methods in Applied Mechanics and Engineering, 191 (2002), 1997--1112.

2. Brown, D. L., Lori Freitag and James Glimm, “Creating interoperable meshing and discretization software: the Terascale Simulation Tools and Technology (sic) Center”, Proceedings of the Eighth International Conference on Numerical Grid Generation in Computational Field Simulations, Waikiki Beach Marriott Resort, Honolulu, Hawaii , June 2-6, 2002.

3. B. Cheng, J. Glimm, X. L. Li and D. H. Sharp, ``Subgrid Models and DNS Studies of Fluid Mixing", Proceedings of the 7th International Conference on the Physics of Compressible Turbulent Mixing, Edited by E. Meshkov, Y. Yanilkin and V. Zhmailo, pp. 385-390, 2001.

4. S. Dutta, E. George, J. Glimm, X. L. Li, A. Marchese, Z.-L. Xu, Y.-M. Zhang, ``Numerical Methods for the Determination of Mixing", Submitted to the 8th International Workshop on Physics of Compressible Turbulent Mixing, 2002.

5. J.B. Drake, D.X. Guo, and Ahmed Khamayseh. "Smooth Grid Transformations with Spectral Methods for Shallow Water Equations" (in preparation)

6. Fann, G., Trease, H., and Trease, L., “Scalable Boundary Grid Generation using Image Processing and CFD-based Methods”, Submitted to SC2002.

7. P. Fast and W.D. Henshaw, "Applications involving moving grids and adaptive mesh refinement on overlapping grids", proceedings of the AIAA Conference on Applied Aerodynamics, June 2001.

8. Flaherty, J.E., Krivodonova, L., Remacle, J.-F. and Shephard, M.S., “Aspects of discontinuous Galerkin methods for hyperbolic conservation laws” Finite Elements in Analysis and Design, 38:889-908, 2002.

9. Flaherty, J.E., Krivodonova, L., Remacle, J.F. and Shephard, M.S., “High-order adaptive and parallel discontinuous Galerkin methods for hyperbolic systems”, WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, p. 1:144, 2002.

10. N. Folwell and P. Knupp, “Sensitivity of Tau3p Cutoff-Time to Mesh Properties,” Stanford Linear Accelerator Technical Report, in preparation.

11. L. Freitag, T. Leurent, P. Knupp, and D. Melander, “MESQUITE Design: Issues in the Development of a Mesh Quality Improvement Toolkit,” p159-168, Proceedings of the 8th Intl. Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, 2002.

12. E. George, J. Glimm, X. L. Li, A. Marchese and Z.-L. Xu, ``A Comparison of Experimental, Theoretical and Numerical simulation Rayleigh-Taylor Instability", Proc. National Academy of Sci., Vol. 99, 5, pp. 2587-2592, 2002.

13. E. George, J. Glimm, J. W. Grove, X. L. Li, Y. J. Liu, Z. L. Xu and N. Zhao),``Simplification, Conservation and Adaptivity in the Front Tracking Method", Submitted to Proceedings of the Ninth International Conference on Hyperbolic Problems Theory, Numeric s, Applications, 2002.

14. J. Glimm, X. L. Li and A. Lin, ``Nonuniform approach to terminal velocity for single mode Rayleigh-Taylor instability", ACTA MATHEMATICAE APPLICATAE SINICA, 18, pp. 1-8, 2002.

15. J. Glimm, X. L. Li and Y.-J. Liu, ``Conservative Front Tracking in One Dimension", Fluid Flow and Transport in Porous Media: Mathematical and Numerical Treatment, Contemprary Mathematics, Edited by Z.-X. Chen and R. Ewing, American Mathematical Society, 295, pp. 253-264, 2002.

16. J. Glimm, X. L. Li, Y. J. Liu and N Zhao), ``Conservative Front Tracking and Level Set Algorithms", Proc. National Academy of Sci., Vol. 98, 25, pp. 14198-14201, 2001.

17. J. Glimm, X. L. Li and Y.-J. Liu, ``Conservative Front Tracking in Higher Space Dimensions" Proceeding of International Workshop on Computational Methods for Continuum Physics and Their Applications, Transaction of NUAA, vol. 18, pp. 1-15, 2001. Submitted for Publication

18. J. Glimm, X. L. Li, Y.-J. Liu and Z. L. Xu, ``Conservative Front Tracking with Improved Accuracy", Submitted to SIAM J. Num Anal., 2001.

19. J. Glimm, J. W. Grove, X. L. Li, Y.-J. Liu and Z.-L. Xu, ``Unstructured grids in 3D and 4D for a time-dependent interface in front tracking with improved accuracy", Submitted to Proceedings of the 8th International Conference on Numerical Grid Generation in Computational Field Simulation, 2002.

20. W.D. Henshaw, "An Algorithm for Projecting Points onto a Patched CAD Model",Proceedings of the 10th International Meshing Roundtable, October 2001

21. W.D. Henshaw, "Generating Composite Overlapping Grids on CAD Geometries", Numerical Grid Generation in Computational Field Simulations, June 2002.

22. W.D. Henshaw, "Overture: an object-oriented framework for overlapping grid applications", Proceedings of the AIAA Conference on Applie d Aerodynamics, June 2001.

23. W.D. Henshaw , "An Algorithm for Projecting Points onto a Patched CAD Model", to appear in Engineering with Computers, 2002.

24. Ahmed Khamayseh and Andrew Kuprat, ``Hybrid Curve Point Distribution Algorithms", SIAM Journal on Scientific Computing, vol. 23, pp. 1464-1484 (2002).

25. Ahmed Khamayseh, Andrew Kuprat, and Paul Henning. "Deterministic Point Inclusion Methods For Boundary Representation Models", SIAM Journal on Scientific Computing, (submitted 2002).

26. Ahmed Khamayseh and Sami Bayyuk. "Gradient-Weighted Adaptive Hybrid Mesh Optimization" (in preparation).

27. Krivodonova, L. and Flaherty, J.E., "Error estimation for discontinuous Galerkin solutions of multidimensional hyperbolic problems," Advances in Computational Mathematics, 2002, to appear.

28. Andrew Kuprat and Ahmed Khamayseh, ``Volume Conserving Smoothing for Piecewise Linear Curves, Surfaces, and Triple Lines'', Journal of Computational Physics, vol. 172, pp. 99-118 (2001).

29. Li, X., Shephard, M.S. and Beall, M.W., "Accounting for curved domains in mesh adaptation", International Journal for Numerical Methods in Engineering, 2002.

30. Luo, X., Shephard, M.S., Remacle, J.-F., O'Bara, R.M., Beall, M.W., Szabó, B.A. and Actis, R., "p-Version Mesh Generation Issues", 11th International Meshing Roundtable, 2002.

31. Luo, X., Shephard, M.S. and Remacle, J.-F., "The Influence of Geometric Approximation on the Accuracy of High Order Methods", Proc. 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Miss. State University, 2002.

32. Neiplocha, J., Trease, H.E., Palmer, B. J., Rector, D.R. (2001). Building an Application Domain Specific Programming Framework for Computational Fluid Dynamics Calculations on Parallel Computers. Tenth SIAM Conference on Parallel Processing for Scientific Computing, March 12-14, 2001.

33. Norris, B., S. Balay, S. Benson, L. Freitag, P. Hovland, L. McInnes, and B. Smith, "Parallel Components for PDEs and Optimization: Some Issues and Experiences", to appear in Parallel Computing.

34. Peterson, N. A. and Kyle K. Chand, "Detecting translation errors in CAD surfaces and preparing geometries for mesh generation", Proceedings of 10th Annual Meshing Round Table, Newport Beach CA, October 2001.

35. Remacle, J.-F., Klass, O., Flaherty, J.E. and Shephard, M.S., "A parallel algorithm oriented mesh database", to appear Engineering with Computers, 2002.

36. Remacle, J.-F. and Shephard, M.S., "An algorithm oriented mesh database", to appear International Journal for Numerical Methods in Engineering, 2002.

37. Remacle, J.-F., Shephard, M.S., Flaherty, J.E. and Klaas, O., "Parallel Algorithm oriented mesh database", Proc. 10th International Meshing Roundtable, Report No. SAND 2001-2976C, pp. 341-349, 2001.

38. Remacle, J.-F., Shephard, M.S. and Flaherty, J.E., “Some issues on distributed mesh representations”, Proc. 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Miss. State University, 2002.

39. Remacle, J.F., Klaas, O. and Shephard, M.S., “Trellis: A framework for adaptive numerical analysis based on multiparadigm programming in C++”, WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, p. 1-164, 2002.

40. Remacle, J.-F., Li, X, Chevaugeon, N. and Shephard, M.S., “Transient mesh adaptation using conforming and non-conforming mesh modifications”, 11th International Meshing Roundtable, 2002.

41. Remacle, J.-F., Flaherty, J.E. and Shephard, M.S., “An efficient local time stepping scheme for transient adaptive calculations”, submitted Comp. Meth. Appl. Mech. Engng., 2001.

42. Remacle, J.-F., Pinchedez, K,. Flaherty, J.E., and Shephard, M.S, “An efficient local time stepping-discontinuous Galerkin scheme for adaptive transient computations, Computer Methods in Applied Mechanics and Engineering, 2001, submitted.

43. Shephard, M.S., Luo, X. and Remacle, J.F., “Meshing for p-version finite element methods”, WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, p. 1-464, 2002.

44. Timchalk, C., Trease, H.E., Trease, L.L., Minard, K.R., and Richard A., “Potential Technology for Studying Dosimetry and Response to Airborne Chemical and Biological Pollutants”, To be submitted 2002.

45. Thomas, S.J., J.M. Dennis, H.M. Tufo, and P.F. Fischer, 2002: A Schwarz preconditioner for the cubed-sphere. Proceedings of the Copper Mountain Conference On Iterative Methods, 2002.

46. Trease, H., Trease, L., Fowler, J., Corley, R., Timchalk, C., Minard, K., and Rommeriem, D., “A Case Study: Extraction, Image Reconstruction, And Mesh Generation From NMR Volume Image Data From F344 Rats For Computational Biology Applications”, 8th International Conference on Grid Generation and Computational Physics, 2002.

6 TSTT Presentations

1. D. L. Brown, “Creating Interoperable Meshing and Discretization Technology, the Terascale Simulation Tools and Technologies Center”, 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, HI, June 2002.

2. D.L. Brown, “The Terascale Simulation Tools and Technologies Center”, Advanced Computing for 21st Century Accelerator Science and Technology Center Kickoff Meeting, Stanford CA, August 2001.

3. D.L. Brown, “The Terascale Simulation Tools and Technologies Center”, A Workshop on the ACTS Collection, Berkeley, CA, September 2002.

4. D. L. Brown, “Overture Software for Solving PDEs in Complex Geometry”, A Workshop on the ACTS Collection, Berkeley, CA, September 2002.

5. K. Chand, "Component Based Hybrid Mesh Generation", Stanford Linear Accelerator Center, Stanford, CA, July 2002.

6. K. Chand, “Overture Tools for Geometry Management and Mesh Generation”, Lawrence Livermore National Laboratory, June 2002.

7. Corley, R.A., Trease, H.E., Minard, K.R., Rommereim, D.N. and Timchalk, C. (2001). Development of a 3-Dimensional, Computational Fluid Dynamics Model of the Respiratory Tract for Evaluating the Dosimetry of Airborne Particulate Matter. Center for Comparative Respiratory Biology and Medicine Pulmonary Seminar Series, University of California, Davis, CA. May 11, 2001.

8. P. Fast, "Overview of NASA's Field Encapsulation Library and implications to design of TSTT Operators, presentation to TSTT team at LLNL, July 2, 2002 .

9. J.E. Flaherty, “Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems,” International Conference on Computational Mathematics, Pohang, South Korea, July 2 - July 5, 2001

10. J.E. Flaherty, “Discontinuous Galerkin Methods for Conservation Laws," Minisymposium on Adaptive Grids in Differential Equations, International Conference on Scientific Computation and Differential Equations, Vancouver, July 29 - August 3, 2001.

11. J.E. Flaherty, “Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems,” Research Institute in Advanced Computer Science (RIACS), NASA Ames Research Center, Moffett Field, January 9, 2002.

12. J.E. Flaherty, “Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems," Institute of Mathematical Sciences, Chinese University of Hong Kong, Hong Kong, March 6, 2002.

13. J.E. Flaherty, “Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems,” Department of Mathematics, State University of New York, Stony Brook, April 17, 2002.

14. J.E. Flaherty, “Adaptive and Parallel Discontinuous Galerkin Methods for Hyperbolic Systems,'” Workshop on Discontinuous Galerkin Methods, Mathematisches Forschungsinstitut Oberwolfach, Oberwolfach, April 22-26, 2002.

15. J.E. Flaherty, “Discontinuous Galerkin Methods for Hyperbolic Systems,” Numerical Analysis Seminar, Courant Institute of Mathematical Sciences, New York University, New York, May 3, 2002.

16. J.E. Flaherty, “Tools for the Adaptive Solution of Problems arising in CFD and MHD,” Minisymposium on Computational Science and Engineering: Tools and Applications, SIAM 50th Anniversary and 2002 Annual Meeting, Philadelphia, July 8-12, 2002.

17. J.E. Flaherty, “Error Estimation for Discontinuous Galerkin Solutions of Hyperbolic Systems,” Minisymposium on Discontinuous Galerkin Methods for Partial Differential Equations, SIAM 50th Anniversary and 2002 Annual Meeting, Philadelphia, July 8-12, 2002.

18. J.E. Flaherty, “Adaptive Software with Biological and Chemical Applications." Symposium in Honor of ICASE's 30th Anniversary, Newport News July 25-26, 2002.

19. P. Fischer, “Spectral Element Methods for Transitional Flows”, Invited presentation at the NCAR Geophysical Turbulence Program workshop "Adaptive and High-Order Methods with Applications in Turbulence", 4-6 February 2002.

20. L. Freitag, “The Terascale Simulation Tools and Technologies Center”, Invited Lecture, Snowmass Accelerator Meeting, Snowmass CO, July 2001.

21. L. Freitag, “Component Technologies for High-Performance Computing”, Invited Seminar presentation, The Pennsylvania State University, State College, PA, October 2001.

22. L. Freitag, “Using Components for Adaptive Algorithms in High Performance Computing Environments”, Invited Keynote, Workshop on Adaptive Algorithms, Mississippi State University, Starksville, MS, January 2002.

23. L. Freitag and P. Knupp, “The TSTT Center and MESQUITE Mesh Quality Improvement Toolkit”, Invited Seminar, Los Alamos National Laboratory, Los Alamos, NM, May 2002.

24. L. Freitag, “Interoperable Meshing and Discretization Technologies”, Invited Seminar, Sandia Naitonal Laboratories, Albuquerque, NM, May 2002.

25. L. Freitag, “TSTT Interface Definition Efforts”, Invited Panel Participant on Meshing and Geometry Standards, International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, HI, June 2002.

26. L. Freitag, “Complex Applications using CCA Technologies”, CCA quarterly tutorial presentations, Santa Fe, January 2002 and Argonne National Laboratory, June 2002.

27. L. Freitag, “The Terascale Simulation Tools and Technologies Center”, SIAM Annual Meeting, Philadelphia, PA, July 2002.

28. L. Freitag, “Interface Definition Efforts in the TSTT Center”, 11th International Meshing Roundtable, Ithaca, NY, September 2002.

29. J. Glimm, August 28, 2001. "Quantification of Uncertainty for Numerical Simulations with Confidence Intervals", Workshop on Uncertainty Quantification, Annapolis MD.

30. J. Glimm, October 11, 2001 "Numerical and Theoretical Methods for the Determination of Mix", High Energy Density Science Symposium, Livermore CA.

31. J. Glimm, December 13, 2001. "Theoretical Methods for the Determination of Mix", Workshop on the Theory of Compressible Turbulent Mixing, Pasadena CA.

32. J. Glimm, January 7, 2002. "Prediction of Oil Production with Confidence Intervals" Workshop on Quantifying Uncertainty and Multiscale Phenomena in Subsurface Processes, Institute for Mathematical Analysis, U. Minn., Minneapolis.

33. J. Glimm, January 15, 2002. "Terascale Simulation Tools and Technologies Center" PIs' Kickoff Meeting for Scientific Discovery with Advanced Computing. Reston, VA.

34. J. Glimm, February 24, 2002. "Mixing in Late Time Supernovae", 4th International Conference on High Energy Density Laboratory Astrophysics, University of Michigan, Ann Arbor, MI.

35. J. Glimm, March 18, 2002. "Recent Developments in (a) Shock Physics Simulations and (b) Prediction with Quantification of Uncertainty". Sandia National Laboratory. Albuquerque, NM.

36. J. Glimm, March 29, 2002. "Predictability and Solution Error Models for Flow in Porous Media". Invited Plenary speaker, Southeast Conference on Partial Differential Equations and Mathematical Physics. U. Alabama, Birmingham AL.

37. J. Glimm, April 3, 2002. "Numerical and Theoretical Methods for the Determination of Mix". Colloquium, Dept. Mechanical Eng. TAMU, College Station TX.

38. J. Glimm, April 10, 2002. "Chaos, complex fluid dynamics and stochastic modeling" Address for VIGRE fellows, U Stony Brook, Stony Brook NY.

39. J. Glimm, April 11, 2002. "Fluids, Numerical Simulation and Applied Mathematics" Stony Brook Mathematics Club. University at Stony Brook, Stony Brook NY.

40. J. Glimm, May 13, 2002. "Numerical and Theoretical Methods for the Determination of Mix" Seminar at Courant Institute of Mathematical Sciences, NYU NY NY.

41. J. Glimm, May 23, 2002. "Engineering 2010: The Plan and the Planning Process", Stony Brook University Chairs' retreat. University at Stony Brook, NY.

42. J. Glimm, June 5, 2002. "Numerical and Theoretical Methods for the Determination of Mix" Plenary talk at the IMPA -- 50 Years Conference. IMPA, Rio De Janeiro, Brazil.

43. J. Glimm, July 9, 2002. "Prediction of Oil Production with Confidence Intervals". Minisymposium talk at SIMA National Meeting, Philadelphia, PA.

44. J. Glimm, August 5, 2002. "Prediction of Oil Production with Confidence Intervals" Invited Plenary Speaker, International Conference on Multiscale Phenomena, Petropolis, Brazil.

45. W.D. Henshaw, "An Algorithm for Projecting Points onto a Patched CAD Model", 10th International Meshing Roundtable, Newport Beach, CA, October 2001

46. W.D. Henshaw, "Generating Composite Overlapping Grids on CAD Geometries", Terascale Simulation Tools and Technologies Mini-Symposium at the 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, HI June 2002

47. W.D. Henshaw, "Overture: an object-oriented framework for overlapping grid applications" Special Session on Overset Tools for AIAA, AIAA Conference on Applied Aerodynamics, St. Louis, MO, June 2001.

48. P. Knupp, "MESQUITE Design," 8th Intl. Conference on Numerical Grid Generation in Computational Field Simulations, 6 June 2002.

49. P. Knupp, "MESQUITE Design," T-Division Colloquium, Los Alamos National Laboratory, 15 May 2002.

50. P. Knupp, "MESQUITE Design and Implementation," Carnegie Mellon Workshop at the 11th International Meshing Roundtable, 18 Sept. 2002.

51. L. Krivodonova, "A Posteriori Error Estimation for Discontinuous Galerkin Method," invited poster presentation, American Women in Mathematics Workshop, SIAM National Meeting, San Diego, July 9 - 13, 2001.

52. L. Krivodonova, "Error Estimation for Discontinuous Galerkin Method," Minisymposium on Discontinuous Galerkin Methods, Sixth U.S. National Congress on Computational Mechanics, Dearborn, August 1 - 3, 2001.

53. Xiaolin Li, "Numerical Tracking of the Material Interface: Why and How", Mechanical Engineering Colloquium, Rutgers University, Oct. 10, 2001

54. Xiaolin Li, "Numerical method in determination of turbulent mixing", 8th International Workshop on Physics of Compressible Turbulent Mixing, Pasadena, CA, Dec. 9-14, 2001.

55. Xiaolin Li, "Simplification, Conservation and Adaptivity in the Front Tracking Method", Invited Presentation, 9th International Conference on Hyperbolic Problems, Theory, Numerics and Applications, Pasadena, CA, March 25-29, 2002.

56. Xiaolin Li, "Unstructured grids in 3D and 4D for a time-dependent interface in front tracking with improved accuracy", 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, Hawaii, June 2-6, 2002.

57. Xiaolin Li, "Front Tracking Method and Fluid Interface Instabilities", CUSPEA Conference on Physics in Twenty First Century, Beijing, June 5-7, 2002.

58. Xiaolin Li, "Simulation of Fuel-injection Jet Using the Front Tracking Method", Colloquium, Department of Mechanics, Beijing University, China, June 7, 2002.

59. Xiaolin Li, "Computational Methods for Partial Differential Equations and Applications", Nanjing Normal University, China, June 13, 2002.

60. Xiaolin Li, “ From Ghost-cell to Conservative Front Tracking”, Minisymposium Presentation at the SIAM 50th Anniversary Meeting, Philadelphia, PA, July 11, 2002.

61. Xiaolin Li, “Ghost-cell to Conservative Front Tracking”,ICM (International Congress of Mathematicians) Satellite Conference on Scientific Computing, Xi'an, China, August 13-18, 2002.

62. Neiplocha, J., Trease, H.E., Palmer, B. J., Rector, D.R. (2001). Building an Application Domain Specific Programming Framework for Computational Fluid Dynamics Calculations on Parallel Computers. Tenth SIAM Conference on Parallel Processing for Scientific Computing, March 12-14, 2001.

63. W. Oh. “A Parallelized, Structured-Unstructured Hybrid, Tetrahedral Grid Construction,” invited presentation to the Department of Mathematics, Pohang University of Science and Technology, Pohang, Korea. August 12, 2002.

64. Remacle, J.-F. “Three Dimensional Parallel Adaptive Discontinuous Galerkin Method for Solving Conservation Laws, Minisymposium on Discontinuous Galerkin Methods, Sixth U.S. National Congress on Computational Mechanics, Dearborn, August 1 - 3, 2001.

65. Remacle, J.-F., “A parallel algorithm oriented mesh database”, 10th International Meshing Roundtable, Newport Beach, CA, Oct. 8, 2001.

66. Remacle, J.-F. “Adaptive Parallel Software for Mesh Management,” Minisymposium on Dynamic Load Balancing for Adaptive Computations, Sixth U.S. National Congress on Computational Mechanics, Dearborn, August 1 - 3, 2001.

67. Remacle, J.F., “Trellis: A framework for adaptive numerical analysis based on multiparadigm programming in C++”, WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, July 8, 2002.

68. Remacle, J.-F., “Higher-order adaptive and parallel discontinuous Galerkin methods for hyperbolic systems”, WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, July 8, 2002.

69. Remacle, J.F., “Parallel Mesh Refinements with Optimal Load Balancing”, WCCM V: Fifth World Congress on Computational Mechanics, Vienna Univ. of Tech, Vienna, Austria, July 10, 2002.

70. Remacle J.F., “Parallel Algorithm Oriented Mesh Datastructure", Adaptive and High-Order Methods with Applications in Turbulence, University of Colorado”, Boulder, February 11-13, 2002.

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98. Trease, H.E., Trease, L.L., Fowler, J.D., NWGrid/NWPhys Workshop and hands-on tutorials, April 2002.

7 The TSTT Team

The TSTT team consists of researchers at six DOE Laboratories and two universities. This sections lists those researchers who were supported by TSTT during FY02, and their levels of effort during that period.

7.1 Argonne National Laboratory

Lori Freitag (25%)

Paul Fischer (25 %)

Henry Tufo (50%)

Thomas Leurent (100%)

7.2 Brookhaven National Laboratory

Jim Glimm (25%)

Wonho Oh (Assistant Scientist, 25%)

Roman Samulyak (Assistant Scientist, 10%)

Myoung-Ngoun Kim (Post Doc, 100%)

7.3 Oak Ridge National Laboratory

Ahmed Khamayseh (0.50FTE)

Valmor de Almeida (0.29FTE)

Ed D'Azevedo (0.09FTE)

7.4 Lawrence Livermore National Laboratory

David Brown 20%

Petri Fast 40%

Bill Henshaw 40%

Brian Miller 20%

Dan Quinlan 25%

Kyle Chand 30%

7.5 Pacific Northwest National Laboratory

Harold Trease (50%)

Lynn Trease (20%)

Manoj Kristman (25%)

Dustin King (UCSD summer student 07-09/2002)

Carmina Armescue (PNNL LTE, supported 06-08/2002)

Programming support (Larry Garhardstien, 5%)

7.6 Rensselaer Polytechnic Institute

Mark S Shephard (Faculty)

Joseph E Flaherty (Faculty)

Dibyendu Datta (Research Staff - partial support)

Christophe Dupre (Research Staff - partial support))

Suleyman Kocak (Research Staff - partial support)

Shrinivas Lankalapalli (Research Staff - partial support)

Yuhua Luo (Research Staff - partial support))

Jean-Francois Remacle (Research Staff - not charged to TSTT)

Eunyoung Seol (Student)

Mohan Nuggehally (Student - started August 2002)

7.7 Sandia National Laboratory

Patrick Knupp (30%)

Tim Tautges (30%)

Darryl Melander (50%)

Mike Brewer (100%)

7.8 State University of New York at Stony Brook

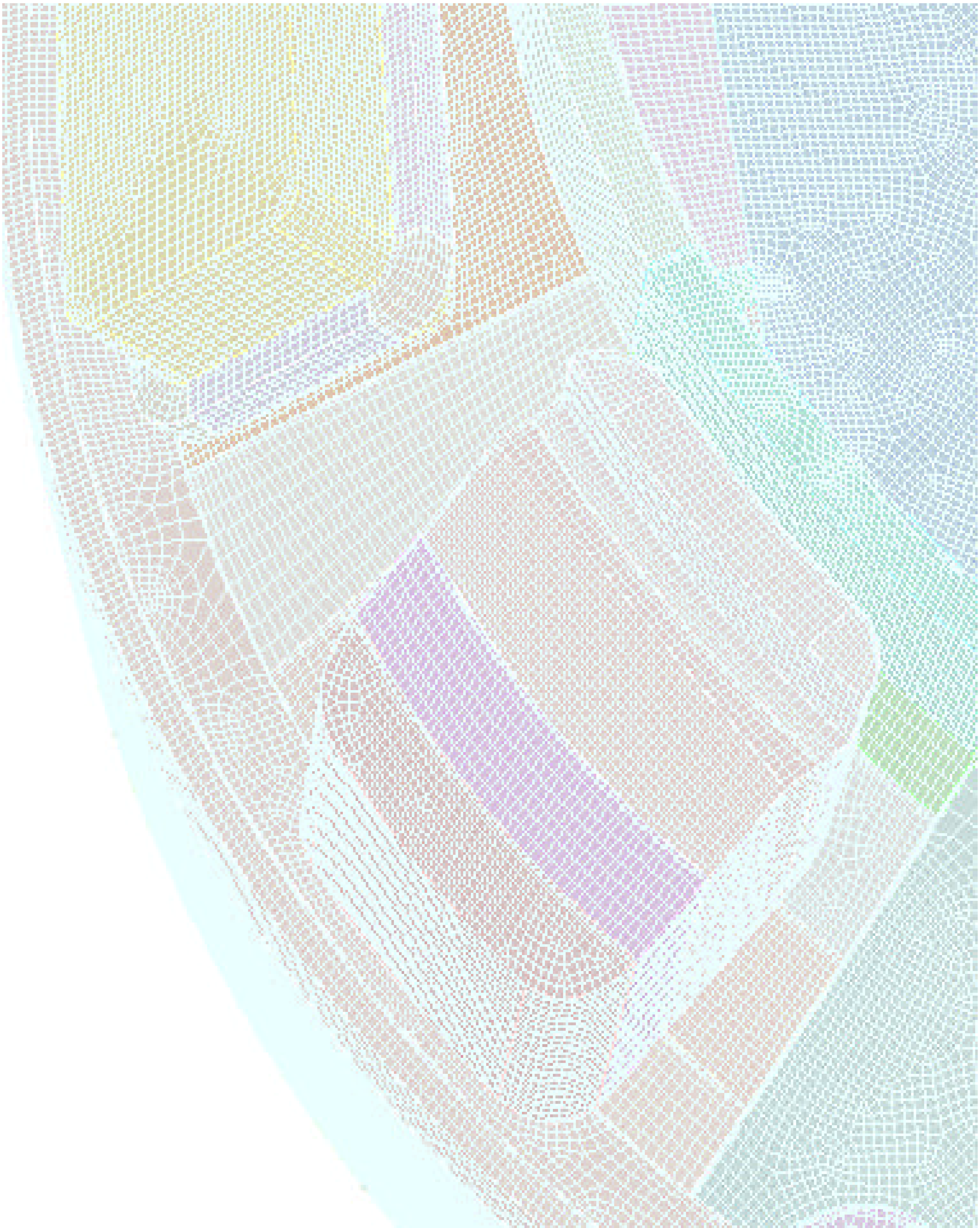
Xiaolin Li (faculty, one summer month)

Ning Zhao (research scientist)

Zhiliang Xu (graduate student)

Yan Yu (graduate student, summer support)

Sohae Chung (graduate student, summer support)



Oak Ridge National Laboratory

Brookhaven National Laboratory

Sandia National Laboratories

Rensselaer

Stony Brook

Pacific Northwest National Laboratory